Computational Methods in Water Resources
XVII International Conference
July 6-10, 2008
Westin San Francisco Market Street Hotel

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A climate driven water resources model

Authors: David Yates, Kathleen Miler, David Purkey

A climate–driven water resource planning model of California's Sacramento River Basin (SACB) is presented, based on the Water Evaluation and Planning model Version 21 (WEAP21). The model's calibration, validation, limitations, and results are presented. The major contribution includes a seamless integration of the watershed's surface and sub-surface hydrology, consumptive and non-consumptive demands, and the water management infrastructure and governance that determine how water naturally flows and is managed. Both supply and demand side interactions are addressed simultaneously, allowing for analysis of alternative and/or future climate scenarios that are unbounded by a reliance on historical hydrologic patterns, with an example shown for the Sacramento river basin.

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A Comparison of Computational Issues for Parameter Estimation using Finite Differences and the Adjoint State Method with MODFLOW and MT3DMS

Authors: Tom Clemo, Michael Fienen

This presentation reports our experiences using both finite differences and the adjoint state method to calculate parameter sensitivities. Neither method is perfectly accurate nor is the finite difference method always continuous with respect to small parameter changes. We explore the influence of those defects on the estimation of hydraulic conductivity of an isthmus separating Crystal and Muskellunge Lakes at the Trout Lake Field Station, Wisconsin. We also explore the influence of intentional manipulation of parameter sensitivity on the parameter estimates. The parameter estimation problem is formulated using a Bayesian approach similar that proposed by Kitanidis (1995). The approach treats hydraulic conductivity as a distributed property that may vary at the scale of the individual model cells. The sensitivity of simulated measurements to nearly every cell in the model is required. Measurements used to constrain the model include hydraulic head, Oxygen 18 fraction, and tritium concentration. Simulation of flow and transport is performed using the MODFLOW-2005 and MT3DMS programs sequentially. An implementation of the adjoint state method for the combined MODFLOW/MT3DMS model has been developed following the approach presented by Samper and Neuman (1986). For a specific change in the hydraulic conductivity, the finite difference calculation is perfectly accurate. The change in simulated measurements is what it is. However, the parameter estimation problem is non-linear making the finite difference sensitivity an approximation to both the parameter change of an update step and to very small parameter changes. The adjoint state method estimates the sensitivity as a continuous derivative of a measurement with respect to the conductivity of a cell. The accuracy of the adjoint state method is limited by the accuracy of the adjoint state solution. The most significant aspect of using the adjoint state method instead of the finite difference approach is over two orders of magnitude reduction in computation time of the sensitivities for our problem. More subtle aspects of the accuracy issues influence the problem through the matrix of sensitivities for the measurements. While the sensitivity matrix is not directly used to establish an acceptable solution of the parameter estimation problem, it does influence the solution through selection of update direction and the final stopping point due to allowances for measurement error. The matrix of sensitivities is also used in the calculation of posterior covariance, and more precision is expected at this point in the algorithm. Nonetheless, significant computational savings may be achieved by limiting the number of times that the most highly accurate sensitivities must be calculated. We explore creative debasement of parameter sensitivities in two ways. One is to reduce very large sensitivities which can lead to improved results. The second is to truncate the adjoint state calculation. This cause a trade-off between computation time and accuracy of the sensitivity calculation.

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A Coupled Biogeochemical Reactive Transport Model for a Riverine Water-Column Benthic sediments

Authors: Arash Massoudieh, Fabian A Bombardelli, Timothy R Ginn

Sediments play a major role in fate and transport of highly sorbing metallic contaminants in water bodies. Sediment-associated contaminants can be released gradually due to diffusive processes, or may be re-entrained in the watercolumn as a result of high flows or anthropogenic activities. In addition biotic and abiotic geochemical transformations in the bed sediments control both the mobility and toxicity of sediment-associated contaminants. Therefore to quantify the fate and transport of contaminants with high affinity to solid particles in water bodies, various processes ranging from hydrodynamic and sediment transport to biogeochemical transformation of contaminants in the sediments need to be considered. In the research being presented, a multi-scale, quasi-two-dimensional, biogeochemical reactive transport model is presented, with description of both theory and numerical implementation. The model includes aqueous water column, suspended sediment, aqueous bed porewater, and sediment bed phases, with associated contaminant transformation and transport, as well as sediment resuspension, deposition and burial. The sediment bed domain is modeled using a set of vertical, Lagrangean (moving with the bed surface) one-dimensional sub-models which take into account burial and compaction as well as diffusive transport and biogeochemical reactions affecting the contaminants. Reactions include speciation, sorption/desorption, and microbially-mediated multiple terminal-electron accepting processes as kinetically-controlled redox reactions. The results of application of the model to simulate the fate and transport of Mercury and its methylation due to activities of sulfate and iron reducing bacteria in Colusa Basin Drain, California will also be presented.

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A Coupled Land Surface-Subsurface Biogeochemical Model for Aqueous and Gaseous Nitrogen Losses Induced by Fertilizer Application

Authors: Chuanhui Gu, Federico Maggi, William Riley, Curt Oldenburg, Norm Miller

A Coupled Land Surface-Subsurface Biogeochemical Model for Aqueous and Gaseous Nitrogen Losses Induced by Fertilizer Application Chuanhui GuTP PT, F. Maggi,P1P W.J. RileyTP PT, N.L.Miller2, C.M. OldenburgP2P Abstract In recent years concern has grown over the contribution of nitrogen (N) fertilizers to nitrate (NOB3PB-P) water pollution and atmospheric pollution of nitrous oxide (NB2BO), nitric oxide (NO), and ammonia (NHB3B). Characterizing the amount and species of N losses is therefore essential in developing a strategy to estimate and mitigate N leaching and emission to the atmosphere. Indeed, transformations of nitrogen depend strongly on water content, soil temperature, and nitrogen concentration. Land surface processes therefore have to be taken into account to properly characterize N biogeochemical cycling. However, most current nitrogen biogeochemical models take the land surface as the upper boundary by lumping the complex processes above the surface as known boundary condtions. In this study, an extant subsurface mechanistic N cycle model (TOUGHREACT-N) was coupled with the community land model (CLM). The resulting coupled model extends the modeling capability of TOUGHREACT-N to include the important energy, momentum, and moisture dynamics provided by CLM. The coupled model showed a significant impact of land-surface diurnal forcing on soil temperature and moisture and on nitrogen fluxes. We also discuss field applications of the model and discuss how temporal dynamics of nitrogen fluxes are affected

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A COUPLED MODELING APPROACH FOR INCORPORATING VARIABLY SATURATED WATER FLOW AND SOLUTE TRANSPORT IN GROUND WATER MODELS

Author: Navin Kumar C. Twarakavi and Jirka Simunek

Owing to the constraints on computational resources, incorporation of variably saturated water flow and solute transport in to ground water models has posed many challenges for ground water modelers in the past. Simplified representation of vadose zone processes in ground water models is a very attractive approach but leads to poor modeling efficiency. A balance between modeling efficiency and computational demand of the adopted approach is thus needed to reasonably represent the effects of vadose zone processes. Recently, the HYDRUS package for MODFLOW has been developed that has been shown to represent vadose zone flow processes in ground water models at different spatial and temporal scales. Here, we extend the capabilities of the HYDRUS package to additionally represent the solute transport in vadose zone. Along with modeling water flow, the new HYDRUS package simulates solute transport such that the MODFLOW-HYDRUS code produce concentrations as a function of time that can be incorporated into the source function for MT3D. The capabilities of the HYDRUS package is tested using examples that represent a variety of spatial and temporal scales.

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A Double Continuum Approach for Two-Phase Flow in Porous Media

Authors: Leopold Stadler, Julia Mayer, Reinhard Hinkelmann, Rainer Helmig

The top soil layers of natural slopes are often highly porous when they consist of numerous macropores. During heavy rainfall, such structures lead to a fast by-passing of water through low permeable layers. Tracer experiments in the field at the natural slope Heumöser Hang in Austria showed the effect of such structures in a fast response of springs on the natural slope. Further investigations figured out that the fast response of the springs was even generated by a complex network of macropores. Such fast infiltration processes play a crucial role for the creeping and failure of hillslopes. For a simulation as close as possible to reality, it is required to describe the complex process interactions of the infiltration with the highly heterogeneous porous structures by accounting for the soil matrix as well as for the macropores. Consequently, this contribution deals with the development of a double continuum model for two-phase flow in porous media. The soil is subdivided into two interacting continua, one representing the soil matrix and the other the macropores. The flow in every continuum is determined by the solution of the two-phase flow equations for two immiscible fluids in a porous medium. Thus, the model concept accounts for the very different flow processes in the soil matrix as well as in the macropores. The exchange fluxes between the continua are described along the macropore surfaces based on a Darcy-type formulation. Therefore, the flow over the macropore surfaces is included in the mass balance equations as a further boundary. Among other things, it is possible to describe the above-metnioned by-passing via macropores during the infiltration with the presented model concept. The double continuum approach is specially suitable for simulations on large scales. The approach leads to a complex system of four coupled non-linear equations. It has been implemented in the modeling system MUFTE-UG. MUFTE is the abbreviation for Multiphase Flow Transport and Energy model and UG for unstructured grids. MUFTE contains physical concepts and discretization methods for multiphase flow and transport processes in porous and fractured-porous media, whereas UG provides data structures and fast solvers based on parallel, adaptive Multigrid methods. The idea of the new approach can be easily transfered into other existing simulation software for flow and transport processes in porous media including modifications for the specific problems. To test the newly developed double continuum approach, several examples have been analysed. As a first example, the displacement of water by a DNAPL (Dense Non-Aqueous Phase Liquid) is investigated because the density difference of the two fluids is small and therefore, this example is numerically \'easier\' compared to other two-phase systems such as water-air. The second example deals with a simplified test case of water infiltration and by-passsing via macropores in an unsaturatedsoil. A third example will treat water infiltration in a natural slope. In the range of possibilities, a comparion of numerical simulations and field measurement will be carried out.

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A Fracture-Only Reservoir Simulator with Physically-Based Transfer Functions

Authors: Evren Unsal, Huiyun Lu, Stephan K Matthai, Martin J Blunt

We propose a simulation methodology that combines the strengths of discrete fracture models with conventional dual porosity simulation. Constructing a grid and solving for flow in both fracture and matrix in a discrete fracture model is frequently so computationally demanding that only small systems can be studied. In contrast, while dual porosity models are more computationally efficient and can be applied at the field scale, they average the fracture properties and the transfer of fluids between fracture and matrix. In our approach we capture the complex geometry and connectivity of the fractures through explicit gridding of the fracture network. However, to avoid the prohibitive computational cost associated with gridding both the fracture and the matrix, we apply transfer functions to accommodate the flow of fluids between these two domains. We use a physically-based approach to modeling the transfer that overcomes many of the limitations of current formulations. The model is based on CSMP, an object-oriented discrete fracture simulator. Only transport in the fractures is considered with fracture/matrix transfer accommodated by source/sink terms associated with each fracture grid block. We discuss how to assign the transfer to account for the physical properties and geometry of the system. We validate the method through comparison with one-dimensional analytical solutions and comparison with experiments and simulations where both fracture and matrix are represented. We then present three-dimensional simulations of multiphase flow in a geologically realistic fracture network. To predict recovery it is necessary to represent the fracture network and the fluid displacement accurately. We discuss the strengths and limitations of our approach and the circumstances under which it is valid.

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A global pressure approach for modelling compressible multiphase flow in heterogenous porous media

Authors: Raphaël DI CHIARA, Gerhard SCHÄFER, Michel QUINTARD, Philippe ACKERER, Guy CHAVENT, Jean-Marie CÔME

A method for the simulation of compressible three-phase flows in heterogeneous porous formations is proposed taking into account gravity, capillary effects and heterogeneity. Governing equations are written in a fractional flow formulation in terms of a global pressure equation and two saturation equations. A global pressure-saturation formulation is much more efficient from the computational point of view than classical approaches in the case where three-phase relative permeability and capillary pressure curves satisfy a total differential (TD) condition as introduced by Chavent & Jaffré (1985). Hence, approximations using current approaches have to deal with two capillary pressure gradients coming from the saturation equations and would therefore require the resolution of four linear systems. However, due to the TD condition, the global formulation requires only the solution of two systems. In the developed approach, the solution of the global pressure equation requires the knowledge of the corresponding three-phase relative permeabilities and the global capillary pressure satisfying the TD condition. In absence of experimental three-phase data, regularity, monotonicity and bound constraints ensure that relative permeabilities are “physical”. Thus, a constrained optimization procedure is used to determine the preliminary secondary variables of the fractional flow from the effective saturation ternary diagram. The obtained three-phase relative permeabilities are compared to those obtained by Stone\'s model. Two efficient numerical methods are used to solve the global pressure equation and the two saturation equations for the water and oil phase. Discontinuous finite elements are used to approximate the convective term of the two saturation equations while the mixed finite element method (with mass lumping) is chosen to solve the global pressure equation and the diffusive part of the saturation equations. In a first test series, we will compare the fully global approach to the pseudo-global approach of Chen and Ewing (1996). Furthermore, the numerical results are compared with analytical two-phase solutions and runs obtained with the multiphase multicomponent simulator SIMUSCOPP (Le Thiez and Ducreux, 1997).

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A level set method for non-zero contact angle drainage and imbibition in realistic porous media

Authors: Masa Prodanovic, Steven L. Bryant

An accurate description of the mechanics of pore level displacement of immiscible fluids could significantly improve the macroscopic parameter predictions such as capillary pressure saturation - interfacial area relationships in real porous media. Slow displacement can be modeled as a quasi-static, capillarity-controlled process. At constant pressure and interfacial tension, pore scale fluid-fluid interfaces are modeled as constant mean curvature surfaces. For a given location in the pore space geometry, such surfaces need not be stable (in which case fluid typically moves until it finds an appropriate location) nor easy to calculate. Further, tracking the topological changes of the interface, such as splitting or merging, is nontrivial. The irregular pore spaces in natural porous media admit a multiplicity of such changes. Assuming quasi-static displacement, we recently developed ([1,2,3]) a simple but robust model based on the level set method for determining fluid interface position during both drainage and imbibition. The original method assumed zero-contact angle and arrived at geometrically correct interfaces. At the same time, the level set based description allows for robust handling of topology changes and independence from the pore space complexity. We now show the extension of the method to handle non-zero contact angles. While slightly more computationally involved than the original, the method preserves the benefits of the level set based description of phases: our simulations establish the exact position and shape of the interface in porous geometries, from which fluid volumes, contact areas and interface curvatures can be readily obtained. We show many examples of 2D and 3D displacements in individual pores (openings) and throat (narrow constrictions), as well as simulations in imaged porous samples and comparison to experimental results. Haines jumps at drainage and pore body imbibition events are readily identified, as well as snap-off and trapping of the non-wetting phase. [1] M. Prodanovic and S. L. Bryant. A level set method for determining critical curvatures for drainage and imbibition. Journal of Colloid and Interface Science, 304 (2006) 442--458. [2] M. Prodanovic and S.L. Bryant. In Focus on Water Resource Research ed. E. Heikkinen, Nova Science Publishers, Hauppage, New York chap. Resolving Meniscus Movement Within Rough Confining Surfaces Via the Level Set Method. (in press) [3] M. Prodanovic and S.L. Bryant. Physics-driven Interface Modeling for Drainage and Imbibition in Fractures. SPE paper 110448, Proceedings of SPE Annual Technical Conference and Exhibition, Anaheim, California, U.S.A., November 2007.

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A mass conservative numerical scheme for reactive solute transport in soil

Authors: Florin Adrian Radu, Sabine Attinger

Environmental pollution of groundwater and soil by organic compounds is nowadays a serious and widespread problem. A comprehensive active remediation often is not feasible from technical or financial reasons. Alternatively, in situ bioremediation (natural attenuation) has been recognized as a promising approach to restore sites contaminated with organic pollutants because it is less costly than active remediation strategies, the contaminants can ultimately be transformed to innoucous by-products with the help of microorganisms (not just transferred to another phase or place) and it can operate in situ. However, the decision to apply natural attenuation at a specific site depends essentially on the reliable prediction of the fate of the contaminant plume. Together with laboratory and field experiments, mathematical models can be used to predict the evolution of a site over long time periods. We present a mass conservative numerical scheme for reactive solute transport in porous media. The transport is modelled by a convection-diffusion-reaction equation, including equilibrium or nonequilibrium sorption. The scheme is based on the mixed finite element method, more precisely the lowest order Raviart-Thomas elements and one-step Euler implicit. The underlying fluid flow is described by the Richards equation, a possible degenerate parabolic equation. A numerical scheme for it was already presented and analysed in [1, 2]. Algorithmic aspects and convergence results will be shown. The scheme is analysed in a general framework, especially taking in account the low regularity of the solution of the Richards equation. An order of convergence estimate is derived which depends on the accuracy of the approximation of the fluid flow. The theoretical results are sustained by relevant numerical studies. REFERENCES [1] F. A. Radu, I. S. Pop, and P. Knabner, Order of convergence estimates for an Euler implicit, mixed finite element discretization of Richards\' equation, SIAM J. Numer. Anal. 42, No. 4, pp.~1452-1478, (2004). [2] F. A. Radu, I. S. Pop, and P. Knabner, Error estimates for a mixed finite element discretization of some degenerate parabolic equations, Numerische Mathematik, to appear, (2008).

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A multicomponent transport and enhanced anaerobic dechlorination model of a single fracture – clay matrix system

Authors: Julie Chambon, Philip John Binning, Poul Løgstrup Bjerg

TCE is a wide spread subsurface contaminant and an important threat to groundwater quality. Many TCE contaminated sites occur in fractured clay systems, and the remediation of these sites is challenging. At such sites, TCE can flow preferentially along fast pathways, formed by the vertical fracture network, and diffuse into the clay matrix. Counter diffusion of TCE to the fracture can take place for hundreds of years after the removal of the contamination source, causing long-term contamination of an underlying aquifer. Recent laboratory and field experiments have shown that bioremediation may be an attractive method for TCE decontamination. Chlorinated solvents can be anaerobically degraded through sequential reactions to a non toxic end product, ethene. Bioremediation, where an electron donor is injected into the fracture system, is a promising remediation strategy that may be able to reduce clean-up times. In order to evaluate remediation potential, a numerical model was constructed to simulate the transport and degradation of TCE in a fracture – clay matrix system. The model is based on field and experimental work including batch and diffusion experiments. The model is an advance on the state of the art as it includes the most up to date knowledge of the sequential degradation processes and involves full coupling between electron donor, biomass and substrate concentrations. The numerical model couples the transport of fluid in the fracture network with diffusive transport in the clay matrix. The model is constructed using Comsol Multiphysics, a generic finite-element partial differential equation solver, and is composed of a single 1D vertical fracture model coupled with a 2D clay matrix model. Equations for TCE and the biodegradation daughter products are written for both the fracture and matrix. The remediation process is simulated by a constant concentration of electron donor in the fracture. The electron donor diffuses slowly into the clay matrix, in order to enhance biodegradation. The sequential dechlorination process, which occurs in the matrix, is modeled with modified Monod's kinetics including limiting substrate and competitive inhibition between the chlorinated ethenes. Monod's kinetics is also used to model growth and decay of biomass in the clay matrix. The numerical model is tested by comparison with batch experimental data for TCE dechlorination and field and experimental data on clay transport and decay. First, site specific results from the batch experiments of reductive TCE dechlorination, in an enrichment culture, using lactate or propionate as electron donor, allow testing the degradation part of the model, including only competitive inhibition and growth and decay of biomass. In a second step, the dechlorination model is tested against field experimental data from a contaminated aquifer. The degradation process was monitored under three different conditions, current site conditions, addition of electron donor (lactate) and addition of both electron donor and dechlorinating biomass. With these data sets, it was possible to test the different components of the degradation model. Finally, the model is tested by comparison with existing approaches, including analytical solutions obtained under simplifying assumptions. The numerical model is employed to simulate the entire history of a contaminated site, including both the contamination phase and subsequent remediation. In the remediation phase, the concentration of TCE and its daughter products is modeled in the clay matrix and at the outlet of the fracture. The amount of substrate, the duration of the injection in the fracture, and the time required to meet the drinking water guidelines at the fracture outlet are assessed. The numerical model allows the formulation and assessment of a complete remediation strategy for TCE contamination in fractured clay based on enhanced anaerobic dechlorination.

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A Multilevel Multiscale Mimetic Method for Two-Phase Flows in Porous Media

Authors: Daniil Svyatskiy, Konstantin Lipnikov, David Moulton

Flow simulations in porous media involve a wide range of strongly coupled scales. The length scale of short and narrow channels is on the order of millimeters, while the size of a simulation domain may be several kilometers. The permeability of rock formations is highly heterogeneous and may span several orders of magnitude, from nearly impermeable barriers to high-permeable flow channels. For such complex systems fully resolved simulations become computationally intractable. To address this problem we developed the new Multilevel Multiscale Mimetic (M^3) method. Using the same mathematical model with averaged parameters to perform simulations at a much coarser scale does not adequately capture the influence of the fine-scale structure. In contrast, the M^3 method constructs a hierarchical sequence of coarse-scale models, which provides a framework to capture fine-scale effects more accurately. Most of existing model upscaling approaches are based on a two-level structure. Using a two-level structure most multiscale methods achieve a coarsening factor of approximately 10 in each coordinate direction, while the trends in finescale realizations of large reservoirs require a coarsening factor of 100 or more. Using the multilevel hierarchy of the M^3 method we achieve large coarsening factors with small computational cost. The M^3 method provides locally conservative velocity fields on all scales, which guarantees local mass conservation. This is a crucial requirement for modeling two-phase flows. Due to its algebraic nature, the method can be adapted to other fine-scale discretizations, such as the Mixed Finite Element and Finite Volume methods, and can handle full permeability tensors and general polygonal meshes. The conservative coarsening procedure is defined by velocity coarsening parameters. These parameters play a critical role in the accuracy of the M^3 method. We implement a black box, problem-dependent, and computationally inexpensive strategy to estimate them. In most multiscale methods the specific parameters that define the coarsening procedure are computed at the initial time step, with high accuracy, and are not changed during the simulation. Our numerical experiments demonstrate that it is important to update these parameters in time, even with moderate accuracy. Thus, we propose to update our velocity coarsening parameters a few times during the simulation (e.g., every 500 time steps) using an efficient algebraic multigrid algorithm with a modest convergence tolerance. With this update strategy the error in the M^3 solution is comparable to the error in the fine-scale solution. The M^3 method has been applied to the upscaling benchmark from the 10th SPE Comparative Solution project. The permeability field has large channelized structures, which is a challenging problem for multiscale methods. To discretize this system in time we use the IMPES time discretization scheme (IMplicit Pressure and Explicit Saturation). The saturation is updated using the Darcy velocities provided by the pressure solver. The numerical results demonstrate that with a large coarsening factor, such as 30, the M^3 solution is close to the fine-scale solution. In other numerical tests for larger problems we implement more aggressive coarsening with a factor of 64, and also observe good agreement with the finescale solution. The M^3 method speeds up the pressure solver up to 80 times, and the overall simulation 8 times, with respect to the fine-scale simulation.

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A multiscale continuum formulation for reactive transport in hierarchical porous media

Authors: Qinjun Kang, Peter C. Lichtner, Partha P. Mukherjee

A multiscale continuum formulation for reactive transport in a hierarchical porous medium is developed. The porous medium consists of a primary continuum coupled to multiple secondary continua either in series or parallel. Multiscale phenomena are captured by taking into account isolated pores described by the secondary continua which are coupled to the primary continuum fluid by diffusion. An analytical solution is derived for the stationary state of a single component system with linear reaction kinetics. This solution is shown mathematically to be equivalent to a single-continuum formulation, with an effective surface area that is a function of the various parameters defining the reactive system. As a consequence it is not possible to directly measure experimentally the effective surface area for the system. One implication of this result is that it provides a possible explanation for the observed discrepancy between field and laboratory measured kinetic rate constants which are based on a single-continuum model interpretation. An example is presented on the basis of a multiscale, synthetic, structured porous medium describing transport of a tracer and linear reaction kinetics.

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A multiscale finite element framework for simulating reactive contaminant transport in heterogeneous porous media

Authors: Kalyana Babu Nakshatrala, Albert Valocchi

Mixing of chemical species across plume boundaries has a major influence upon reactive pollutant fate in the subsurface. Small-scale heterogeneity leads to irregular plume boundaries which enhances mixing-controlled reactions through increasing the interfacial area of the plume. Therefore, it is crucial to capture this small-scale heterogeneity in order to properly model reactive transport. Unfortunately, computational limitations do not permit full resolution of the smallest scales of heterogeneity, and thus it is necessary to use a coarse numerical grid, particularly for cases with a large number of reactive species. In order to capture the sub-grid scale heterogeneity effects, we present two multiscale methods for reactive contaminant transport. Multiscale finite element methods have been proven successful for diffusion and Darcy flow problems, and we extend two popular methods to advective-diffusive reactive system. We report our preliminary studies for steady state fast bi-molecular reactions. The first method is based on the multi-scale decomposition of the solution, and is an extension of the numerical subgrid upscaling method NSUM proposed by Arbogast [1] (which has been applied to Darcy flow). The governing system is divided into two sub-problems – coarse-scale and finescale. The concentration of each chemical species is split into two components – coarse-scale (which is defined at the grid scale) and fine-scale (which is defined at the smallest modeled scale). The fine-scale sub-problems are solved locally by constructing numerical Green's functions, which are independent of the coarse-scale problem. The localization of fine-scale sub-problems is achieved by the closure assumption, which in our case is the prescription of homogeneous Dirichlet boundary condition for the fine-scale sub-problem. The second multiscale method constructs special shape functions that capture the underlying small-scale information. This method is an extension of the multiscale finite element method (MsFEM) proposed by Hou and Wu [2]. We generate basis functions by solving homogeneous advection-diffusion equation with heterogeneous velocity and permeability in each element. With proper choice of boundary conditions, these basis functions form a partition of unity. One uses these special functions as shape functions. Finally, we compare the numerical solutions obtained using the proposed multiscale finite element methods on both model and realistic problems.
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A new approach for hydrogeological modeling in discretely-fractured media: from 3D geological representation to numerical simulations

Authors: Blessent Daniela, Therrien René

A new approach to simulate fluid flow and solute transport in discretely-fractured media has been developed by coupling the HydroGeoSphere numerical code (Therrien et al. 2005) with the mesh generation software LaGriT (Los Alamos National Laboratory) and by representing complex fractured geological formation with the 3D geological modeling platform GOCAD (Mira Geoscience). GOCAD is an advanced software designed to visualize and edit 3D geological objects that are discretized with different geometrical entities, such as points, segments and facets. Since a discrete fracture conceptual model is used, each fracture is explicitly defined by its own geometry and then discretized with 2D finite elements. The surrounding rock matrix, which can be porous and contribute to flow or transport, is discretized with 3D finite elements. For the fractures and matrix, 2D triangles and 3D tetrahedra are chosen because they are the most flexible elements to handle complex geometrical domains that are typical of fractured geological formations. The first step of the approach presented here uses the GOCAD platform to represent fractures as 2D non planar triangulated surfaces in the 3D space. If two surfaces intersect each other, a conforming triangulation at their intersection is needed. In the next step, GOCAD surface files are imported in the LaGriT mesh generation software. To integrate triangulated fracture surfaces within 3D tetrahedral elements representing the rock matrix, a background hexahedral mesh is built. This mesh is basically used to develop a regular point distribution inside the simulation domain and it can be easily refined where required, for example around fractures. All nodes belonging to the hexahedral mesh and to the triangulated fracture surfaces are then copied to a new mesh object and connected to form a 3D tetrahedral mesh. Original fracture surfaces can be extracted from the tetrahedral mesh, together with their connectivity information. The method also ensures that each triangle lying on a fracture surface corresponds to the face of a surrounding tetrahedron. The resulting 3D tetrahedral mesh generated by LaGriT, as well as the triangular fracture meshes, is finally directly read by the HydroGeoSphere code, which performs all calculations with tetrahedral and triangular elements. Illustrative examples have been designed to verify and validate the approach. These examples show that the proposed spatial discretization can reproduce solute propagation along fractures more accurately than other fracture discretization configurations, which tend to lengthen fracture pathways. The reason is that fractures, which can be planar or not, are built and discretized with their actual path length. Simulation results for simple scenarios are also compared to existing analytical solutions. Although complex 3D meshes can be generated, the approach allows for easy refinement around fractures, representing a great asset for the accuracy of the numerical solution. In addition, simulations show that the total CPU time is only slightly increased by using a tetrahedral mesh, making the use of this kind of mesh to represent complex geometries a more suitable choice compared to blocks or prisms based meshes. In conclusion, the examples show that this mesh generation approach and the improved HydroGeoSphere version constitute a new suitable and more realistic way to investigate fractured geological media.

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A new mixed finite element method on hexahedra, its equivalent sparse finite volume formulation, and convergence of multipoint flux approximations in 3D

Authors: Sebastien F. Matringe, Ruben Juanes, Hamdi A. Tchelepi

Multipoint flux approximation (MPFA) methods are finite volume methods that approximate the vector variable (the flux) through interfaces as a linear combination of a scalar variable (the pressure) evaluated at the centers of all the surrounding gridcells. These methods are used to discretize of the second-order elliptic problem on distorted or unstructured grids with full-tensor coefficients. The MPFA O-method [1] is implemented in virtually all petroleum reservoir simulators but a proof of its convergence remains elusive for 3D hexahedral grids. Russell and Wheeler [2] established the equivalence between traditional finite differences and mixed finite elements (MFE) based on the lowest order Raviart–Thomas space (RT0) with quadrature. Arbogast et al. [3] extended this work to tensor coefficients in 3D using an expanded MFE method, that discretizes the scalar, its gradient, and the vector variable. Unfortunately, there is severe loss of accuracy for discontinuous coefficients. Klausen and Winther [4] proved convergence of the MPFA O-method in 2D by means of a broken RT0 space. Recently, Wheeler and Yotov [5] used the first order Brezzi-Douglas-Marini space (BDM1) and a quadrature to prove convergence of MPFA for triangular and quadrilateral elements and 3D tetrahedra. 3D hexahedra were not considered. The difficulty in extending this approach to hexahedra is to obtain a vector space conforming in H(div) and that localizes to a finite volume method under appropriate quadrature. Here, we present a new vector space defined on the reference hexahedron that is conforming in H(div) and that has four degrees of freedom per face [7]. The new space is constructed by enriching the space of linear polynomials by divergence-free polynomials of higher degree. The new velocity space is compatible with a constant pressure space to define a consistent and convergent MFE method. In addition, the MFE method is localized into the MPFA O-method by the application of the trapezoidal quadrature. Thus, we prove, for the first time, convergence of the MPFA O-method on 3D rectangular hexahedra [8]. We obtain optimal error estimates for the new MFE and for the MPFA O-method in both the scalar and vector variables. These results are confirmed by numerical convergence studies. References [1] I. Aavatsmark. An introduction to multipoint flux approximations for quadrilateral grids. Comput. Geosci., 6:405–432, 2002. [2] T. F. Russell and M. F. Wheeler. Finite element and finite difference methods for continuous flows in porous media. In R. E. Ewing, editor, The Mathematics of Reservoir Simulation, pages 35–106. SIAM, Philadelphia, PA, 1983. [3] T. Arbogast, M. F. Wheeler, and I. Yotov. Mixed finite elements for elliptic problems with tensor coefficients as cell-centered finite differences. SIAM J. Numer. Anal., 34:828–852, 1997. [4] R. A. Klausen and R. Winther. Convergence of multipoint flux approximations on quadrilateral grids. Numer. Methods Partial Differential Equations, 22(6):1438–1454, 2006. [5] M. F. Wheeler and I. Yotov. A multipoint flux mixed finite element method. SIAM J. Numer. Anal., 44(5):2082–2106, 2006. [6] S. F. Matringe, R. Juanes, and H. A. Tchelepi. Streamline tracing for general triangular and quadrilateral grids. Soc. Pet. Eng. J., 12(2):217—233, 2007. [7] S. F. Matringe, R. Juanes, and H. A. Tchelepi. Mixed finite element and related control volume discretizations for reservoir simulation on three-dimensional unstructured grids. In SPE Reservoir Simulation Symposium, Houston, TX, February 26–28 2007. (SPE 106117 – Submitted to Soc. Pet. Eng. J.) [8] S. F. Matringe, R. Juanes, and H. A. Tchelepi. A new mixed finite element on hexahedra that reduces to a cell-centered finite difference method. Numer. Math., 2007. (Submitted).

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A Parallel and Adaptive Algorithm for Computation of Shallow Water Flows

Authors: Eli Atetjevich, Peter O. Schwartz, Dan Graves, Julie Percelay, Qiang Shu, Phil Colella

Water resource management in the Sacramento-San Joaquin Delta requires hydrodynamic and water simulation over large, multi-scale domains with complex geometry. Often problems must be solved over a variety of hydrologic conditions, in which case simulations are long and performance-bound. We are developing a 2D hydrodynamic model for a shallow water estuary that is designed for multi-processor computation using a Cartesian mesh, embedded boundaries (Cartesian cut cells) to conform to bathymetry and the natural boundaries of the system, and adaptive mesh refinement (AMR) for efficient handling of multi-scale problems. The Cartesian solver is based on a second order Godunov algorithm with a Corner Transport Upwind correction of fluxes to achieve better resolution in directions oblique to the grid. Due to its shock-capturing properties, this algorithm has the potential to achieve superior results in transient problems such as flood flows. The stability problems of small cut cells are handled by hybridizing the conservative discretization with a stable, non-conservative discretization at irregular cells, with the result that local accuracy and stability depends only on the dimensions of the larger Cartesian grid cells.We present the formulation of our model, testing results, geometry processing techniques and an application in the Bay Delta. We also describe the institutional setting in which we intend to use and further develop the model and how this affects our design. In the future, our work will be extended to moving boundary problems such as intertidal wetting and drying and flooding, particle transport and three dimensional modeling.

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A parallel-computing method for modeling large-scale groundwater flow

Authors: Dong Yanhui, Guomin Li

Though many advancements and refinements of the computational methods have been achieved over the last decade, large-scale simulation of ground water flow in complicated geological formations remains a challenge. Many problems arise from computational efforts required for solving large sparse-matrix systems. High-performance, parallel-computing techniques, being increasingly used for computationally-intensive scientific applications, are a powerful tool to modeling large-scale ground water flow. In the paper, a parallel solver for MODFLOW2000 is developed for solving large-scale groundwater flow. The parallel solver is based on PCG(Preconditioned Conjugate-Gradient) Package of MODFLOW2000 with OpenMP Application Program Interface (API). And then, PGFSA, a 3D parallel simulator based on a code named GFSA(Li Guomin, 1994) is developed combining Message Passing Interface (MPI) and OpenMP. Simulation results show that the parallel-computing technique enhances modeling capability efficiently in speedup of computing times for large-scale modeling studies. Citation: Arlen W. Harbaugh et. al. 2000, Modflow-2000, the U.S. Geological Survey Modular Ground-Water Model-User Guide to Modularization Concepts and the Ground-Water Flow Process, U.S. Geological Survey Open-File Report 00-92;Michael J. Quinn, Parallel Programming in C with MPI and OpenMP, EISBN: 0-07-282256-2; Mary C. Hill 1990, Preconditioned Conjugate-Gradient 2 (PCG2), a Computer Program for Solving Ground-Water Flow Equations, U.S. Geological Survey Water-Resources Investigations Report 90-4048.

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A path forward for biogeochemical reactive transport modeling of in situ uranium bioremediation

Authors: Steven Yabusaki & Philip Long, Yilin Fang, Mary Lipton, Jill Banfield, Robert Hettich, Nathan VerBerkmoes, Lee Kerkhof, Derek Lovley, Darrell Chandler, Aaron Peacock

Ongoing bioremediation research has shown that subsurface uranium immobilization can be achieved in situ by stimulating indigenous metal reducing bacteria with electron donor amendments. Reliable, cost-effective uranium bioremediation in the field will require the development of a systematic and quantitative predictive understanding of the complex linkages between hydrology, geochemistry, and microbiology. Yet, identifying appropriate conceptual process models and unraveling interactions between processes under dynamic and variable hydrologic and geochemical conditions is a significant scientific challenge. We present a development path for integrating microbial processes into a field-scale, multicomponent biogeochemical reactive transport simulation capability that is part of a research project on long-term uranium immobilization at a U.S. DOE, Office of Science Integrated Field Challenge (IFC) Site. The characterization of the microbiological processes at this site is based on gene expression, proteogenomic analysis, stable isotope probing, and phospholipid fatty acid profiles. Under the IFC, focused microarrays and analysis systems are being developed to provide near real-time, in-field mRNA and protein assays to identify temporal and spatial changes in microbial community composition and activity before, during, and after biostimulation. Coupling the growth, metabolism, and function of the dominant microbial populations with concomitant changes in the subsurface biogeochemistry provides a basis for assessing and developing mechanistic process models. Information obtained from microbial assessment techniques and their use in the simulation capability are described below. The cellular concentration of expressed genes over time provides a measure of how individual species are adapting their structure and function to the electron donor amendment and the evolving biogeochemical environment. Gene expression data provides a direct measure of the potential rate of Fe and U reduction that can be compared with U removal rates. Information on up regulation or down regulation of specific genes can provide new knowledge on the conditions controlling the onset and termination of TEAPs as well as microbial function kinetics at different stages of the field bioremediation. Proteogenomic approaches, based on the integration of metagenomic and proteomic data, provide a means to define the strain and species makeup of samples and to track temporal and spatial changes in microbial activity levels. The protein complement can be monitored at the strain level as cells proliferate and TEAP is utilized. Proteogenomics methodologies for relatively complex natural consortia, for which only partly representative isolate genomes are available, are only now being developed, but initial results from the IFC are promising and are expected to yield insights that will directly inform the modeling process. Stable isotope probing will be used to follow labeled carbon in the electron donor amendment through the microbial community over time. This will allow the identification of the principal microorganisms responsible for consuming the electron donor in the initial stages of the biostimulation, quantification of biomass yield for these microorganisms, and, in later stages, identification of predation and/or utilization of decaying biomass by succeeding populations. As our ability to assess the metabolic state of microorganisms in the context of changing biogeochemistry advances, we foresee an evolution to more robust, quantitative linkages to the stoichiometry of biologically mediated reactions and associated rate laws. Comprehensive, large-scale simulation of field-scale experiments can then provide a framework to evaluate the scale-up of the fundamental mechanisms, and identify the conditions where these mechanisms will be important under field conditions.

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A PILOT TEST OF CO2 SEQUESTRATION IN A DEPLETED GAS FIELD IN THE PO PLAIN, ITALY: FLUID-DYNAMICAL AND GEO-MECHANICAL ISSUES

Authors: Massimiliano Ferronato, Giuseppe Gambolati, Carlo Janna, Pietro Teatini

The 1997 Kyoto protocol prescribes for the agreeing nations a reduction of the carbon dioxide emission to the atmosphere that for Italy should be in prospective as much as 100 Mt/y by 2012. Geological CO2 sequestration in deep geological formations can help fulfill this requirement. The potential to store large CO2 quantity is offered by gas reservoirs (either in production or depleted) and saline aquifers. A pilot project of CO2 sequestration in a depleted gas field located in the sedimentary basin underlying the Po river plain, northern Italy, is under planning. The reservoir is formed by a gentle anticline about 1400 m deep and surrounded by an active aquifer. Sealed by a 200 m thick impermeable formation, the geologic unit of interest is made of several sandy/clayey sequences bounded by regional faults and crossed by a number of local fractures. The field development started in 1950, was practically completed in the mid \'70s, and since the early \'90s the reservoir is used for hydrocarbon storage. The pilot test consists of injecting 8000 t/year of CO2 over 3 years. A numerical study is performed to explore the extent of migration of the injected CO2 plume and investigate the geo-mechanical aspects related to the safety of sequestration, i.e. possible pre-existing fault activation, caprock fracturing, and ground surface uplift induced by changes in the effective stress. The simulations are carried out with the aid of finite element / interface element codes for the geo-mechanical simulations. A number of parametric scenarios are analyzed to address the major uncertainties concerning the location of the injection well, the geomechanical properties of the sedimentary sequence, and the natural stress regime. The results show that the pilot test is quite safe from the geo-mechanical viewpoint.

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A Reactive Transport Model for Lactate Stimulated Hexavalent Chromium Reduction at Hanford 100H Site

Authors: Sumit Mukhopadhyay, Eric L. Sonnenthal, Boris A. Faybishenko, Susan S. Hubbard

Lawrence Berkeley National Laboratory and Pacific Northwest Laboratory are collaborating on a project to perform field-scale investigations of biostimulation of hexavalent chromium, Cr(VI), reduction at the DOE Hanford 100H site in Washington. Biostimulation for Cr(VI) reduction with HRC® (Hydrogen Release Compound), produced by Regenesis, is based on stimulating the natural microbial population to induce a dynamic process of biogeochemical transformation in the subsurface. The goal is to reduce Cr(VI) to the trivalent state, which precipitates as chromite [Cr(OH)3(s)], thus removing toxic Cr(VI) from groundwater. HRC is a polylactate polymer bonded that slowly releases lactic acid after injection into an aquifer. HRC thus acts as a long-time electron donor and carbon source for native bacteria that stimulate Cr(VI) reduction to the trivalent state. This process occurs either directly, where Cr(VI) acts as terminal electron acceptor for specific subsurface microbes, or indirectly, where the addition of lactate (via HRC) to the aquifer causes the microbial population to remove oxygen, nitrate, sulfate and other competing electron acceptors and depress the redox potential. Species thus produced also include ferrous iron and sulfide. Changes to the subsurface caused by biostimulation may include such processes as dissolution and precipitation of minerals, surface complexation, generation of gas, changes in soil water content and oxygen concentration, sorption, attachment/detachment, oxidation and reduction, biofilm generation, and changes in permeability and effective porosity. We are developing a reactive transport model to investigate the lactate-induced reduction of Cr(VI) in the groundwater of the Hanford 100H aquifer. The ultimate objective of the modeling activity is to investigate some or all of the biogeochemical processes described above with respect to lactate-induced Cr(VI) reduction in groundwater. In this paper, however, we focus on the impact of certain geochemical reactions (such as goethite reduction to Fe(II) and subsequent reduction of CR(VI) by FE(II); impact of bicarbonate on the extent of CR(VI) reduction, etc.) controlling Cr(VI) reduction in groundwater. The numerical model is based on the TOUGHREACT reactive geochemical transport software [Xu et al., 2006]. The model domain included three-dimensional heterogeneous saturated Hanford sediments. Spatial distribution of hydraulic conductivity was obtained through geophysical measurements [Hubbard et al., 2006]. The grid is extremely refined and radial near the injection and pumping wells, but is rectangular and less refined farther away from these wells. HRC was injected through an injection well, and groundwater was pumped from a monitoring well situated about 5 m away from the injection well. The flow model (i.e., without reactive transport) was constrained against Br tracer injection test data. We compare simulated time-series of Cr(VI) in the dissolved phase with measured Cr(VI) field data. Modeling confirms that FE(II) has a strong impact on the extent of Cr(VI) reduction. In addition, since it is assumed that the model domain is located in the saturated zone, no separate gas phase was present. Consequently, carbon dioxide produced during the reaction was accounted for as dissolved bicarbonates (HCO3-). This resulted in an oversaturation with HCO3- (as no carbon dioxide could leave the model domain), ultimately resulting in an underprediction of Cr(VI) reduction. We are thus currently extending the model to include an unsaturated zone and other biogeochemical processes.

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A Scientific Data Repository Based on Ontology Design

Authors: Amanda Hines, Dr. Chris Bogen

Over the past few years computer simulations have gained wider acceptance as viable alternatives to field testing. Due to this recognition, the numbers of simulations and types of simulations have increased significantly. This increase in computational modeling has produced the need for access to large amounts of data in a short amount of time. Also, it is not uncommon for data requirements to change at any moment, especially in a research environment such as the US Army Engineer Research and Development Center (ERDC). The ERDC recognized the need for a centralized, scientific data repository. It was essential for this repository to be easily accessible to users and flexible enough to handle the range of data required by the modelers. This presentation will discuss the repository, iSciDat, which has been created to address these issues at the ERDC. At the design stage and throughout the implementation of iSciDat, modelers were contacted to provide input about the process. Initially, these modelers were from the groundwater and surface-water fields. Based on their input, the repository's initial functionality was to store soil properties. After obtaining a list from the modelers, these properties were generated inside iSciDat. However, due to the evolving nature of research, the list has grown and will continue to grow. The best-equipped people to add or change these properties are the modelers themselves. This presented a dilemma since most modelers are not database experts. Therefore, the repository had to be created with enough flexibility that the modelers could easily manage the data definitions and relationships on their own. With this as the major driving force for design, we determined that an ontology-based repository was the best option. Ontologies provide the flexibility and hierarchical structure needed for this environment. This implementation of the repository allows modelers full control of their data storage without the daily need of a database manager and it also provides accessibility to store and retrieve data through the Internet. This presentation will discuss in depth the design rationale and implementation for the ERDC repository iSciDat.

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A series solution for multi-layer aquifers with natural geometry

Authors: Sanders Wong, James R. Craig

An analytical solution has been developed for a two-dimensional steady-state saturated groundwater flow system with multiple layers of arbitrary geometry. Each layer has a unique hydraulic conductivity value, and there is no limitation upon the number of layers included in the model. Similar to Toth's solution (Toth, J., A theoretical analysis of groundwater flow in small drainage basins, J. Geophys. Res., 67, p4795-4812, 1963), the system is enclosed on the bottom and sides by no-flow boundary conditions; a known configuration of the water table leads to a specified-head condition along the top of model. The analytical series solution is obtained by maintaining flow and head continuity across each interface by minimizing the sum of squared errors at a set of control points. The specified head condition at the water table is treated similarly. Similar to Read (Read, W.W., Series solutions for Laplace's equation with nonhomogeneous mixed boundary conditions and irregular boundaries, Math. Comput. Modelling, 17(12), p9-19, 1993), the geometry of each layer can be represented using arbitrary continuous geometric functions, e.g., Fourier series or splines. The method will be demonstrated via application to two-layer and multi-layer aquifer systems with different arbitrary shapes of the water table, bottom boundary, and layer interfaces. The solution, implemented in Matlab, is computationally inexpensive, highly accurate, and, unlike numerical solutions, is easily reconfigured for different geometries and performs well for very low height-to-length ratios.

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A Stochastic-Lagrangian Model for Multiphase Flow in Porous Media: Upscaling of Non-Equilibrium Pore Scale Dynamics

Authors: Manav Tyagi, Patrick Jenny, Hamdi A Tchelepi

CO2 storage in subsurface formations involves many complex physical processes that are well understood at the pore scale. However, in a real scenarios, it is not feasible to perform pore scale simulations, and one needs a large scale model. Unfortunately, the Darcy based large scale models for multiphase flow and transport are questionable, particularly in the context of CO2 storage. One of the main assumptions in these models is the concept of relative permeability and capillary pressure, which are expressed as functions of saturation. Moreover, these quantities are typically measured under equilibrium conditions and scale independence is assumed. However, under unstable conditions these assumptions may not be valid. We proposed [1] an alternative modeling approach based on the Lagrangian movement of stochastic particles, which represent infinitesimal fluid phase volumes and evolve such that their statistics represent the statistics of the actual fluid volumes. Each particle is labeled by a fluid phase, has its individual velocity, a position in physical space and possibly other properties, e.g. CO2 concentration. As a particle moves in physical space, its properties change according to the stochastic processes such that the specified Lagrangian statistics is honored. The goal of this work is to model these stochastic processes based on the pore scale physics. For the illustration purpose a simplified 3D pore-network consisting of spherical pores and cylindrical throats is considered. The flow through the network is described by simple rules for the fluid movement in the throats and for the pore filling [2]. First, flow with self-similar average saturation profiles are investigated. These cases correspond to multiphase Darcy flow, where the relative permeabilities are uniquely determined by the saturation values. More interesting are those scenarios, where no self-similar profile can observed and classical multiphase Darcy model fails. For such cases non-equilibrium phenomena at the pore scale play an important role and we demonstrate how these can be modeled in our stochastic particle framework. With the help of pore-network simulations first the non-equilibrium pore scale dynamics has been studied. Then, based on the extracted Lagrangian statistics, comparative simulations with stochastic particle method have been performed.
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A study of vortices in shallow water with BGK algorithm

Authors: Man Yue, Lam, Hongwei, Liu, Mohamed S. Ghidaoui

Large scale vortices with vertical axis and which extend from the bed to the water surface are common in shallow water flows. For example, such vortices can be found in the wake of islands, in the downstream of headlands and other protrusions, at the confluence of two streams with differing speeds (e.g., channel junction), in compound and composite channel, etc. This paper conducts numerical experiments in order to investigate the origin of the vortices and their growth in scale as well as their sensitivity to inflow perturbation, Froude number and bottom friction. The numerical model used is based on the finite volume approach where the fluxes are determined from the Boltzmann Bhatnagar-Gross-Krook (BGK) (Ghidaoui et al. 2001). The BGK scheme is second order in both time and space, conserves both mass and momentum, satisfies the entropy condition and has been previously applied to various hydraulic problems including bores, oblique hydraulic jumps, tidal waves and shallow mixing layers. References: Ghidaoui, M. S., Deng, J. Q., Gray, W. G., Xu, K. 2001 A Boltzmann based model for open channel flows. Int. J. Numer. Meth. Fluids, 35, 449-494

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A survey on non-negative numerical formulations for tensorial diffusion equations

Authors: Kalyana Babu Nakshatrala, Albert Valocchi

Robustness of numerical methods for flow and transport problems in porous media is important for development of simulators to be used in a wide range for applications in subsurface hydrology and contaminant transport. Obtaining non-negative solutions on unstructured meshes along with local and global mass balance is a particularly essential feature in the simulation of reactive transport of contaminants since the nonlinear reaction term leads to nonsensical unstable solutions for negative concentrations. The heterogeneity in the velocity field will give rise to a non-homogeneous anisotropic dispersion tensor with non-negligible cross terms. Several studies have shown that standard treatment of the cross-dispersion term will result in non-positive solutions on general computational grids. Several ad-hoc methods have been proposed in the literature. For example, a post processing step is performed in which one does some sort of "smoothing". But this procedure, in many cases, will violate mass balance. Some other methods are limited in their range of applicability (e.g., the method can handle only structured grids, etc.). Herein we consider only the dispersion/diffusion process for steady single-phase flow in heterogeneous anisotropic porous media. Such a flow can be described by the Poisson's equation with a tensorial diffusion coefficient, which when written in the mixed form is similar to the Darcy equations. We survey various popular numerical formulations from both the finite element and finite volume literature, and comment on their numerical performance with respect to the following metrics: • what are the restrictions on mesh and medium properties to obtain non-negative solutions, • whether the method exhibits local and global mass balance, • what is the accuracy of the method for smooth problems, and • can the method handle unstructured 2D and 3D grids (not just logically rectangular grids)? An ideal formulation is the one that exhibits local and global mass balance, second-order accuracy for smooth problems, and unconditionally produces non-negative solutions on unstructured meshes. From the finite element literature we consider – the classical single-field Galerkin formulation, Raviart-Thomas element, stabilized mixed formulation based on the variational multiscale, stabilized mixed discontinuous Galerkin formulation. From the finite volume literature we consider – multi-point flux approximations (MPFA) proposed by Aavatsmark and co-workers, the formulation by Herrera and Valocchi [1], and a new nonlinear two-point finite volume method proposed by Lipnikov and co-workers [2]. We provide general guidelines based upon the robustness of each method, the ease of programming, flexibility for incorporating advection and transient conditions, and computational efficiency. References [1] P. Herrera and A. Valocchi. Positive solution of two-dimensional solute transport in heterogeneous aquifers. Ground Water, 44:803–813, 2006. [2] K. Lipnikov, M. Shashkov, D. Svyatskiy, and Y. Vassilevski. Monotone finite volume schemes for diffusion equations on unstructured triangular and shape-regular polygonal meshes. Journal of Computational Physics, 227:492–512, 2007.

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A Thermodynamically-Based Model For Predicting Microbial Growth And Community Composition Coupled To System Geochemistry

Authors: Jonathan D. Istok

'Bioimmobilization' of redox-sensitive metals and radionuclides is being investigated as a way to remediate contaminated groundwater and sediments. In this approach, growth-limiting substrates are added to stimulate the activity of targeted groups of indigenous microorganisms and create conditions favorable for the microbially-mediated precipitation ('bioimmobilization') of targeted contaminants. We present an approach for modeling this process that couples thermodynamic descriptions for microbial growth with associated geochemical reactions. A synthetic microbial community is defined as a collection of defined microbial groups; each with a growth equation derived from bioenergetic principles. The growth equations and standard-state free energy yields are appended to a thermodynamic database for geochemical reactions and the combined equations are solved simultaneously to predict the effect of added substrates on microbial biomass, community composition, and system geochemistry. This approach, with a single set of thermodynamic parameters (one for each growth equation), was used to predict the results of laboratory and field bioimmobilization experiments at two geochemically diverse research sites. Predicted effects of ethanol or acetate addition on uranium and technetium solubility, major ion geochemistry, mineralogy, microbial biomass and community composition were in general agreement with experimental observations although the available experimental data precluded rigorous model testing. Model simulations provide insight into the long-standing difficulty in transferring experimental results from the laboratory to the field and from one field site to the next, especially if the form, concentration, or delivery of growth substrate is varied from one experiment to the next. Although originally developed for use in better understanding bioimmobilization of uranium and technetium via reductive precipitation, the modeling approach is potentially useful for exploring the coupling of microbial growth and geochemical reactions in a variety of basic and applied biotechnology research settings.

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A variational multiscale high-resolution method for the simulation of unstable multiphase flow in heterogeneous formations

Authors: Francois-Xavier Dub, Luis Cueto-Felgueroso, Ruben Juanes

Multiscale phenomena are ubiquitous to flow and transport in porous media. They manifest themselves through at least the following three facets: (1) effective parameters in the governing equations are scale dependent; (2) some features of the flow (especially sharp fronts and boundary layers) cannot be resolved on practical computational grids; and (3) dominant physical processes may be different at different scales. Numerical methods should therefore reflect the multiscale character of the solution. We concentrate on the development of simulation techniques that account for the heterogeneity present in realistic reservoirs, and have the ability to solve for coupled pressure-saturation problems (on coarse grids). We express the governing equations of multiphase flow as a pressure equation (of near-elliptic nature) and a saturation equation (quasi-hyperbolic equation). Both are nonlinear, but only weakly coupled. We propose a variational multiscale (VMS) method for the solution of the pressure equation, which splits the original problem rigorously into a coarse-scale problem and a subgrid-scale problem. A high-order finite volume method is used to solve the saturation equation. The proposed VMS method employs a low-order mixed finite element method at the coarse scale, and a finite volume method at the subgrid scale. We identify a weak compatibility condition that allows for subgrid communication across element interfaces, which turns out to be essential for obtaining high-quality solutions. We also introduce an effective, locally conservative formulation of multiscale sources (wells) that relies on a decomposition of fine-scale source terms into coarse and deviatoric components, and on the definition of multiscale “well” basis functions. The saturation equation is then solved on the fine scale by a high-resolution explicit finite difference method. In the course of the simulation, adaptivity is used to minimize the number of shape functions that need to be updated for the solution of the pressure equation. The proposed approach provides highly accurate solutions to flow scenarios that display viscous fingering and channeling, with challenging permeability fields and concentrated fine-scale source terms.

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Adaptive Kronrod-Patterson integration of highly non-linear element matrices

Authors: Hans Janssen

Current adaptive mesh-refinement approaches – be it r-, h- or p-based – all seek to minimise the deviation between a reference solution and the actual discretised solution. The deviation between reference and discretised solution may arise from two sources: deviation due to the inaccurate discretised representation of the continuous fields of independent variables – the discretisation error –, and deviation due to the inaccurate numerical integration of the element storage and transfer matrix coefficients – the integration error. Most adaptive mesh-refinement approaches resolve mesh regions with too large deviations by addition (h/p-based adaptivity) of discretisation nodes, some by relocation (r-based adaptivity). It is hence implicitly assumed that the discretisation error dominates the deviation from the reference solution. For linear PDE's, with constant storage and transfer coefficients, this assumption is most likely valid. PDE's describing variably saturated subsurface or building material moisture transfer are however highly non-linear: the moisture capacity and permeability of building materials might vary some ten orders of magnitude from dryness to saturation. For such PDE's, the actual discretisation may be sufficient to accurately represent the continuous fields of independent variables, but not to accurately integrate the elements' storage and transport matrices. While such deficient numerical integration may of course be resolved by local densification of discretisation nodes (mesh-refinement), this comes at the price of extra degrees of freedom in the system and a complex mesh-refinement algorithm. An alternative technique, directly targeting the integration error, is presented here. It equally allows to enhance the numerical fidelity of flow and transport simulations, however with a minimal implementational and computational expense, while moreover being complementary to adaptive mesh-refinement approaches. In the first section, the dominance of the integration error in the accuracy of simulation of moisture transfer in building materials will be exemplified. To that goal, one-dimensional and two-dimensional simulations of moisture absorption and drying are performed, with monotonously coarsening discretisations. It will be verified that the deviation from the reference solution is strongly dependent on the order of the used numerical integration scheme, confirming the dominance of the integration error. As it is unnecessary and uneconomical to apply high-order integration for each and every element in the discretisation, an adaptive strategy will be put forward. To that aim, the recursive Kronrod-Patterson numerical integration scheme is implemented with an a posteriori error criterion on the resulting values of the element's storage and transport matrices. The investigation will show that such adaptive approach provides the right balance between computational accuracy and expense. In a final section a more pragmatic and computationally inexpensive simplification will be presented, applying an a priori estimation of the required integration order, based on the expected variation of the parameters in the element's storage and transport matrices. It will be demonstrated that, if correctly calibrated, it yields similar results at an even lower computational cost. While the study here is limited to single-phase moisture transfer in porous building materials and the general finite-element method without mesh-adaptation, the presented principle is equally applicable for other strongly non-linear transport phenomena and in more advanced finite element approaches, as well as in other discretisation schemes making use of numerical integration.

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Adaptive Markov Chain Monte Carlo Sampling and High Performance Computing for Estimating Parameters in High-Resolution Three-Dimensional Flow and Transport Models

Authors: Jasper A. Vrugt, Bruce A. Robinson, Cajo ter Braak

Markov chain Monte Carlo (MCMC) methods have found widespread use in many fields of study to estimate the average properties of complex systems, and for posterior inference in a Bayesian framework. Existing theory and experiments prove convergence of well constructed MCMC schemes to the appropriate limiting distribution under a variety of different conditions. In practice, however this convergence is often observed to be disturbingly slow. This is frequently caused by an inappropriate selection of the proposal distribution used to generate trial moves in the Markov Chain. I this talk, I will show that significant improvements to the efficiency of MCMC simulation can be made by using a self adaptive Differential Evolution learning strategy within a population based evolutionary framework. This scheme, entitled DiffeRential Evolution Adaptive Metropolis or DREAM, runs multiple different chains simultaneously for global exploration, and automatically tunes the scale and orientation of the proposal distribution during the search. I will demonstrate the advantages of DREAM using several synthetic benchmark problems, including a real-world study involving the estimation of permeability and dispersion parameters in a high resolution three-dimensional flow and particle tracking model using Magnetic Resonance Imaging (MRI) data of a conservative tracer moving through a flow cell. This inverse problem is solved using high performance computing with 100 different computational nodes.

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Adaptive multiscale finite element method for subsurface flow simulation.

Authors: J.M. van Esch, F.B.J. Barends

Natural geological formations generally show multiscale structural and functional heterogeneity evolving over many orders of magnitude in space and time. In subsurface hydrological simulations the geological model focuses on the structural hierarchy of physical subunits and the flow model addresses the functional hierarchy of the flow process. Flow quantities like pressure, flux and dissipation relate to each other by constitutive relations and subunit parameters like porosity and hydraulic permeability. Hydraulic permeability includes the (steady state) intrinsic permeability and the (time dependent) relative permeability for unsaturated conditions. Laboratory experiments provide measurements of the subunit parameters on the fine scale. The intrinsic permeability is the most dominant parameter and the most heterogeneous parameter affecting the fluid flow on the field scale. In general constitutive relations change for different scales. However, for the multiscale problem under investigation, Darcy's law is supposed to remain valid on both laboratory scale and field scale. If laboratory measurements are treated stochastically within the geological model, then the structural model of the subsurface should be built on the same scale as these supporting measurements. Fully resolved flow simulations on this scale are intractable and a new multiscale technique has been developed. The newly developed adaptive multiscale finite element method extends the original two-level multiscale finite element method to a hierarchy of scales. The multiscale finite element method captures the fine scale behavior on a coarse mesh by multiscale basis functions. Originally the weights of the multiscale basis functions follow from a local flow simulation. The local flow problems are closed by dimensionally reduced flow computation results. In this form the method forms a class of subdomain decomposition techniques and suitable for parallel computation. Variational multigrid methods implicitly construct multiscale basis functions if certain restrictions on the interpolation operator are satisfied. The set of basis functions is defined recursively from the finest level as multigrid operates on a predefined grid hierarchy. The newly developed method applies variational coarsening. At first a multistep coarsening procedure provides a separation of fine grid unknowns and coarse grid unknowns on triangular and tetrahedral elements and constructs a local intergrid transfer operator. The coefficients of the transfer operator, which resemble the weights of the multiscale basis functions, follow from a dimensionally reduced flow problem. Secondly multiscale homogenization extracts the effective permeability tensor from the multiscale basis functions in a pre-calculation phase. The homogenization procedure resembles pressure-dissipation averaging on local flow problems. The effective permeability is not unique and depends on the local boundary conditions. An upscaling criterion detects parts of the domain where averaged permeability tensors may be used on (static) coarse elements, and subsequently the number of integration points can be reduced. Finally adaptive grid refinement concentrates the computational work on localized phenomena like sinks and in infiltration fronts. On the (dynamically) refined parts downscaling of the permeability takes place. A mesh regularization algorithm eliminates non-conforming elements. The parallel implementation of the adaptive multiscale finite element algorithm solves transient partly saturated subsurface flow problem effectively. This will be illustrated by a case study.

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An Accuracy Evaluation of the Parallel Adaptive Hydrology (ADH) Program for Unsaturated Flow Using Analytical Solutions

Authors: Fred T. Tracy, Stacy E. Howington

The parallel Adaptive Hydrology (ADH) finite element computer program has become the standard for many Engineer Research and Development Center (ERDC) flow simulations. One such application is unsaturated flow. Because real-world problems are so complex, testing codes such as ADH for accuracy is often difficult. This is particularly true when flow is in the vadose zone where Richards' equation is highly nonlinear. Recently, however, Tracy (2006 and 2007) has derived analytical solutions for a box-shaped flow region that is initially very dry until water is applied to the top of the region. This includes two-dimensional (2-D) and three-dimensional (3-D) solutions for steady-state and transient flow with two specified head equations for the top and either specified head or no-flow boundary conditions for the sides of the soil sample. This gives eight scenarios. The bottom of the soil sample remains very dry. Further, this totally unsaturated flow problem can be made more and more nonlinear and thus stress the nonlinear and linear solvers in ADH as much as needed by simply changing a parameter α. The purpose of this work is to test ADH using the above described analytical solutions for various values of α and determine the error in the computations for certain strategic node points. It has been shown using other computational schemes that the errors grow rapidly with the same grid size and time-step size as the problem becomes more nonlinear, and the nonlinear solver often struggles to converge at all. The following are examples of aspects of accuracy that will be considered: (a) effect of grid size, (b) effect of time-step size, (c) effect of nonlinearity as represented by α, (d) robustness of the Newton nonlinear solver and the bi-conjugate gradient stabilized (BiCGSTAB) linear solver with its different preconditioners, (e) effect of "upwinding" the relative hydraulic conductivity computation as compared with using an average value for the element, and (f) effect of increasing the number of processors in the parallel environment. Comparison of results with other groundwater programs will also be made. Both 2- and 3-D analytical solutions will be used in the test. The 2-D solution in the 3-D ADH code will be tested by doing a vertical cross section with a layer of elements in the third direction having the thickness of the grid spacing Δ. In fact, each hexahedron of grid size Δ × Δ × Δ is divided into six tetrahedral elements. - REFERENCES - Tracy, F. T. (2006). "Clean Two- and Three-Dimensional Analytical Solutions of Richards' Equation for Testing Numerical Solvers." Water Resources Research, 42, W08503. - Tracy, F. T. (2007). \"Three-Dimensional Analytical Solutions of Richards' Equation for a Box-Shaped Soil Sample with Piecewise-Constant Head Boundary Conditions on the Top." Journal of Hydrology, 336, Issues 3-4, 7 April 2007.

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An Adaptive Multiscale Finite Volume Formulation for Two-phase Flow and Transport in Porous Media

Authors: Hui Zhou, Seong Lee, Hamdi Tchelepi

Recent advances in multiscale methods have shown great promise in efficiently simulating multiphase flow in heterogeneous media with high resolution. However, existing multiscale methods only solve the flow equations for pressure in a multiscale approach. Saturation in transport equations is usually solved in fine scale, which takes a large portion of CPU cost especially when flow equations are solved with efficient adaptive multiscale approaches. The main difficulty in multiscale modeling of transport equations lies in the nonlocal memory effect in homogenizing a hyperbolic convection equation. The problem is further complicated by the complex interactions between saturation, flow, and spatial heterogeneity in immiscible displacements. We developed an adaptive multiscale finite-volume (MSFV) method for the transport equation of nonlinear two-phase flow in heterogeneous domains. The objective here is not to develop an upscaled (coarse-scale) operator for the transport equation because of the complex interactions between saturation, flow, and spatial heterogeneity in immiscible displacements. Instead, an adaptive reconstruction strategy is developed. The method can be described using prolongation and restriction operators as in a two-level multigrid scheme. The restriction operator is defined as the volume average of the fine-scale saturations in a coarse block. Three adaptive prolongation operators are defined according to the saturation distribution, in which the physical domain is divided into three regions: (1) Region 1 where the injection fluid has not arrived, (2) Region 2, where steep saturation gradients are present, and (3) Region 3 where saturations change slowly in the wake of advancing front. To identify the transition between the regions, specific norm-based criteria are proposed. In Region 1, the transport equation can be completely skipped, whereas in the Regions 2 the local fine-scale transport equations are solved iteratively on a coarse grid (this is referred as Prolongation Operator I). In Regions 3, we developed two approximate prolongation operators: Prolongation Operator II that reconstructs the fine-scale velocity and is locally conservative on the fine grid, and Prolongation Operator III that interpolates saturation changes to yield a locally conservative scheme, but only on the coarse grid. The proposed adaptive multiscale method has been tested with various models, including systems with strong permeability heterogeneity. The results demonstrate clearly that the multi-scale results with adaptive transport calculations are in excellent agreement with the fine-scale reference solutions. Furthermore, the adaptive scheme for coupled flow transport equations yields solutions that are much more computationally efficient than conventional finite difference methods.

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AN ENSEMBLE APPROACH TO VARIATIONAL DATA ASSIMILATION

Authors: Arnold Heemink, Muhammed Umer Altaf

Data assimilation methods are used to combine the results of a large scale numerical model with the measurement information available in order to obtain an optimal reconstruction of the dynamic behavior of the model state. Variational data assimilation or the adjoint method has been used very often for data assimilation. This approach is especially attractive for model calibration problems. Using the available data, the uncertain parameters in the model are identified by minimizing a certain cost function that measures the difference between the model results and the data. In order to obtain a computational efficient procedure, the minimization is performed with a gradient-based algorithm where the gradient is determined by solving the adjoint problem. Variational data assimilation requires the implementation of the adjoint model. Even with the use of the adjoint compilers that have become available recently this is a tremendous programming effort, that hampers new applications of the method. Therefore we propose a new approach to variational data assimilation using model reduction that does not require the implementation of the adjoint of (the tangent linear approximation of) the original model. Model reduced variational data assimilation is based upon a POD (Proper Orthogonal Decomposition) approach to determine a reduced model for the adjoint of the tangent linear approximation of the original nonlinear forward model. Using an ensemble of forward model simulations an approximation of the covariance matrix of the model variability is determined. A limited number of leading eigenvectors (EOFs) of this matrix are selected to define a model sub space. By projecting the original model onto this subspace an approximate linear model is obtained. Once this reduced model is available, its adjoint can be implemented very easily and the minimization process can be solved completely in reduced space with negligible computational costs. If necessary, the procedure can be repeated a few times by generating new ensembles more close to the most recent estimate of the parameters. Compared with the classical variational method the adjoint of the tangent linear model is replaced by the adjoint of a linear reduced forward model. The model reduced approach is solving exactly the same optimization problem, but since the adjoints are different, the gradients of the criterion will be different too and the optimization process will probably terminate in different local minima. Model reduced variational data assimilation tends to be more robust than the classical approach. While the adjoint of the tangent linear approximation of the original model produces the exact local gradient, the model reduction approach is based on a statistically linearized model and produces a spatially averaged gradient. As a result the model reduced approach is less sensitive for local minima. In the presentation we will introduce the ensemble approach to variational data assimilation. The characteristics and performance of the methods will be illustrated with a number of real life data assimilation applications in groun water flow models and coastal sea models.

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An Integrated Hydrology/Hydraulic and Water Quality Model for Watershed-scale Simulations

Authors: Cheng Wang, Gour-Tsyh Yeh, Fan Zhang, Guobiao Huang

This paper presents a first principle, physics-based watershed-scale model of integrated hydrology/hydraulic and water quality transport, WASH123D 3.0. This numerical model comprises of three modules: (1) one-dimensional (1-D) simulation module, which is capable of simulating coupled fluid flow, sediment transport and reactive chemical transport and transformation in river/stream networks; (2) two-dimensional (2-D) simulation module, capable of simulating coupled fluid flow, sediment transport, and reactive chemical transport and transformation in two-dimensional overland flow systems; and (3) three-dimensional (3-D) simulation module, capable of simulating coupled fluid flow and reactive chemical transport and transformation in three-dimensional variably saturated subsurface systems. The Saint Venant equation and its simplified versions (diffusion wave and kinematic wave forms) are employed for surface fluid flow simulations and the modified Richards equation is applied for subsurface flow. These governing equations are solved with several physically and mathematically based numerical options. In the transport simulations, fast/equilibrium reactions are decoupled from slow/kinetic reactions with the decomposition of reaction networks, which enables robust numerical integrations. Kinetic variables are adopted as primary dependent variables rather than biogeochemical species to reduce the number of transport equations and simplify reaction terms. In each time step, hydrologic/hydraulic variables are solved in the flow module, kinetic variables are then solved in the transport module. This is followed by solving the reactive chemical system node by node to yield concentrations of all species. In order to obtain accurate, efficient and robust computations, five numerical options are provided to solve the advective-dispersive transport equations and three coupling strategies are employed to deal with the reactive chemistry. Application examples will be presented to demonstrate the design capability of the model. This model may be of interest for the environmental scientists, engineers and decision makers as a comprehensive assessment tool to reliably predict the fluid flow and sediment and contaminant transport on watershed scales so as to evaluate the efficacy of alternative watershed management and remediation techniques prior to incurring expense in the field.

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An integrated model of G. sulfurreducens for investigating bioremediation of U(VI) in subsurface sediments

Authors: Srinath Garg, Radhakrishnan Mahadevan, Timothy Scheibe, Yilin Fang, Philip Long, Derek Lovley

Metals (e.g., chromium, mercury) and radionuclides (e.g., uranium, strontium) are major subsurface contaminants in many US Department of Energy (DOE) facilities. These elements possess high mobility in subsurface environments, and are long lived due to their long half-life periods, and pose a potential risk to humans and the natural environment. In-situ bioremediation is being studied as a potent and powerful technology for remediation of uranium at DOE wastes. This method focuses on the microbial mediated reduction of uranium from soluble U(VI) valence state to the relatively insoluble U(IV) valence state. Since elemental uranium cannot be degraded into daughter products, current research focuses on making use of this radionuclide as an electron acceptor in microbial respiratory processes. In-situ bioremediation can be implemented by introducing a soluble electron donor (e.g., acetate), thereby stimulating the in-situ activity of dissimilatory metal reducing organisms such as G. sulfurreducens. In order to optimize the subsurface bioremediation strategy for maintaining long-term activity of Geobacter species, a framework integrating the genome-scale metabolic model and transport process was developed and numerical simulations of bacterial U(VI) reduction in subsurface sediments were carried out. This model incorporates the flow of groundwater under anaerobic conditions and the dynamics of growth and respiration of G. sulfurreducens with acetate as the electron donor and iron and uranium as the electron acceptors. In contrast to existing models of bioremediation, the new framework accounts for changes in microbial function (respiratory pathways) in response to local geochemical conditions through application of a constraint-based in silico modeling method. Two uses of the in silico model are tested: 1) incorporation of modified microbial growth yield coefficients based on the in silico model, and 2) variation of reaction rates in a reactive transport model based on in silico modeling of a range of local geochemical conditions. Preliminary results from this integrated model will be presented.

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An iterative multiscale finite-volume method converging to the fine-scale solution

Authors: Ivan Lunati, Seong H. Lee

The Multiscale Finite-Volume (MSFV) method has been originally developed to efficiently solve homogenous (zero right hand side) elliptic problems on large domains with highly heterogeneous coefficients. The MSFV algorithm has been employed to solve the pressure problem in a pressure-saturation formulation of multiphase flow in porous media. An auxiliary coarse grid (defining the control volumes) is employed, together with its dual, to solve a coarse-scale pressure problem. A set of local numerical solutions on dual cells (basis functions) is used to interpolate the coarse-grid pressure and obtain an approximate fine-scale pressure distribution. Then the saturation problem is solved by a standard Schwarz overlap solution method. Recently, some modifications of the original algorithm have been proposed that allow modeling physically complex flow, e.g., multiphase flow at the presence of gravity and capillary forces (or even the black-oil flow). In this framework, an additional local solution per dual cell is used to correctly capture the effects of the additional physical mechanisms, which appear on the right hand side of the pressure equation. This local solution (correction function) can be regarded as a particular solution of the localized problem, the superimposition of the basis functions being the general solution. Given the localization assumption the definition of basis and correction functions is straightforward and the splitting can be carried out rigorously. For the case of gravity-driven flow, numerical simulations demonstrate excellent agreement between the MSFV solutions for pressure and saturation and the corresponding fine-scale reference solutions. Note, however, that the accuracy of the MSFV solutions depends on the quality of the localization. To improve the boundary conditions of the local problems, hence, the accuracy of the MSFV solution, we develop an iterative scheme and we discuss its similarities with domain decomposition methods. Note that introducing the correction function is essential to obtain an algorithm converging to the fine-scale solution.

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An openMI-coupled surface-subsurface flow simulation model sys-tem to forecast subsurface flood

Authors: Becker, Bernhard, Reuter, Christian, Schuettrumpf, Holger

The problem of groundwater head rise in urban regions due to river stage rise and inundation during flood water has been reported in several current studies. Groundwater head rise may affect subsurface buildings like underground rail tunnels and cellars and cause flooding of depressed areas or areas be-hind dikes. For some urban regions, site specific groundwater models and inundation models for surface flow already exist. For the case study, we already have a 2D horizontal groundwater model, which has been developed for water supply purpose. This site-specific model is based on the finite element groundwa-ter flow program FEFLOW (DHI-WASY). Also, a 2D storage cell inundation model being used for estimating the danger of flooding in the urban areas exists. For both models, the river stage forms the main boundary conditions. In order to obtain a forecasting tool for operational purpose in „subsurface flood“ protection, these two models shall be coupled iteratively using the openMI standard (www.openmi.org). The challenge in coupling the two models is to make the programs openMI compliant. Usually this requires changes in the source code: the program has to be reorganized to be compiled as a dynamic linked library (dll), and basic program functions must be made available for openMI. Being a commercial program, the source code of FEFLOW is not available for this survey. But FE-FLOW provides a programming interface which allows the user to implement own code into the flow simulation. We show how we made FEFLOW an openMI compliant using this programming interface. The FEFLOW interface and the openMI classes are linked with c++ remote procedure calls and dot net platform invoke routines. The use of existing models in a subsurface flood forecasting modeling system is appropriate due to the following reasons: firstly, no extra site-specific models have to be set up. This reduces the work load for the development of the modeling system, and verification and validation work only needs to be focused on the coupling procedure. Secondly, the forecasting model always will represent the best updated state, because the model components are maintained separately by the authorities who devel-oped them and use them. Thirdly, a high degree of acceptance is achieved when users of the subsur-face modeling system can work with programs and models they already know. In the end, using the openMI standard provides high flexibility for future expansions.

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Analysis of Mixed Explicit-Implicit Method

Authors: Amir Riaz, Romain de Loubens , Hamdi Tchelepi

Efficiency of explicit time integration schemes is limited substantially when the local CFL number varies by orders of magnitude in different regions of the computational domain. Fully implicit schemes allow larger time steps but suffer from excessive numerical dispersion. Higher order spatial discretization can be combined with a fully implicit scheme to minimize the error, however, this approach is also computationally expensive. We present a mixed explicit-implicit finite volume method that retains the benefits of both schemes by reducing the computational cost of higher order schemes through adaptive selection of a small number of fully implicit cells (Adaptive Implicit Method). We show that a $O(\\Delta x)$ error occurs at the boundaries of implicit-explicit cells and propose a new numerical treatment to remove the error. Extensive 2D calculations for miscible and two-phase Darcy flow are carried out to determine the practical feasibility of our adaptive scheme as well as to demonstrate the improvement in accuracy, that is significant in some cases, over conventional low order schemes.

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Analysis of the interplay between contaminant transport scales, aquifer heterogeneity and health related parameters in a risk-driven approach for site characterization

Authors: Felipe P. J. de Barros, Yoram Rubin, Reed Maxwell

Understanding the role of model parameters in a human health risk assessment due to groundwater contamination may aid decision makers in defining better allocation of resources. Due to our inability to fully characterize the subsurface, it becomes extremely important to develop data acquisition strategies that will best contribute to uncertainty reduction in the final risk. It is of our interest to identify flow and transport conditions in which parametric uncertainty reduction will lead to better estimates of adverse health effects. Furthermore, being able to understand the worth of information from hydrogeological parameters, when counter-balanced with uncertainty and variability in human physiological response and behavioral parameters, may prove useful in defining characterization efforts. By making use of the available computational tools and through a consistent methodology, we investigate the impact of site characterization in the final risk estimates. Simulations are repeated for several different physical conditions such as plume ergodicity, the scale of the capture zone and levels of aquifer heterogeneity. Results indicate that the value of hydrogeological information is dependent on the interplay between length scales of the plume, dimensions of the capture zone and the scale of the screen in which the water is being sampled. The methodology accounts for uncertainty and variability in the risk-related parameters. Sensitivity of model predictions is also investigated for different physiological dose-response models.

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Analysis of the split operator approach for multispecies reactive transport models

Authors: Babak Shafei, Philippe Van Cappellen

Analysis of the split operator approach for multispecies reactive transport models: Mixed kinetic and equilibrium reactions Reactive transport models (RTMs) are powerful tools to estimate the fate and transport of chemical constituents. They can be developed to simulate interactions between fluids and solids in porous media through physical and chemical processes. In most cases these interactions involve multi-component chemical systems which introduce multiple unknown species concentrations and nonlinearity in the system. Therefore, multiple advection-dispersion-reaction equations (ADRE) need to be solved simultaneously. Split operator (OS) methods are in widespread use for the numerical solution of coupled nonlinear reactive transport problems. The advantages of OS algorithms come with the cost of the truncation error. Previously developed error analyses have focused on relatively single reaction systems including, for example, unimolecular or bimolecular kinetic reactions, or nonlinear equilibrium adsorption isotherms. An error analysis for OS applied to realistic multispecies and multidimensional reactive transport models considering mixed kinetic and equilibrium reactions is presented. The derived error expression can be applied to a variety of chemical processes taking place in the subsurface such as aqueous complexation, oxidation-reduction reactions, mineral dissolution-precipitation, acid-base equilibria and sorption and ion exchange. The error analysis is illustrated for multi-component reaction networks with particular attention for the errors on concentrations of chemical species participating in different types of reactions (kinetic, equilibrium or both of them). It is shown that when the error related to the effect of the boundary condition (by assuming homogeneous boundary condition) is neglected, the error in the model domain depends on the transport regime (advection or diffusion). Errors in the OS method are compared to those of the fully implicit solution and the differences are discussed.

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Analytical and Numerical Properties of the Diffusive Wave Approximation of the Shallow Water Equations with Applications to Water Flow in Wetlands.

Authors: Mauricio Santillana, Clint Dawson

In this work we address the quantitative and qualitative aspects of modeling water flow driven mainly by gravitational forces and dominated by shear stress, i.e. under uniform and fully developed turbulent flow conditions. These particular flow regimes are present in marshes, wetlands and many estuaries. The effective equation that has been recently used to simulate these particular flow regimes is a doubly nonlinear and degenerate diffusion equation. This equation is often referred to in the literature as the diffusive wave approximation of the shallow water equations (DSW) and it is obtained by approximating the depth averaged continuity equations by empirical laws such as Manning's or Chezy's formulas and then combining the resulting expression with the free surface boundary condition. The DSW equation contains as particular cases the Porous Medium equation and the p-Laplacian. In this study we present key characteristics of the solutions of the initial/boundary value problem arising from this equation along with suitable numerical methods aimed at approximating them. We focus our attention in obtaining physical solutions of the DSW equation using the Galerkin method and present a priori error estimates between the true solution and the Galerkin approximate solutions. We present as well some examples where an unstructured-grid finite element code was implemented to solve the DSW equation and used to simulate water flow on real experimental settings as well as real environments.

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APPLICATION OF 2-D COMPUTER MODEL IN RESERVOIR DEVELOPMENT – A CASE STUDY FROM INDIA

Authors: Dr.S.K.Sharma

[Funding dependent abstract - I, being from India need and request for travel grants to participate]. Geothermal exploration carried out in India, so far, has generated valuable data through extensive surface, earth scientific studies backed-up by exploratory drilling down to the depths of about 500 meters at selected geothermal localities concerning structural, geological, geochemical, hydrological and thermal parameters of geothermal systems. One such site is the Tattapani Geothermal Field situated in Surguja district of Chattisgarh. Under the geothermal exploration program for experimental utilization of heat from thermal fluids, as many as 26 boreholes were drilled for depths varying from 100 meters to 620 meters in an area of about 2 Km2. Drilling of these boreholes was completed during April - December, 1993 by the Geological Survey of India (GSI). The GSI has reported that only five boreholes have been planned as production wells which were producing a cumulative hot water at the rate of 60 liters per second (lt/s) at about 1000C. These parameters indicate the possibilities of electric generation from low to medium enthalpy reservoir with the help of binary power plants based upon the Organic Rankine Cycle (ORC). The potential of the field has further been assessed using conceptual model developed for computer simulation exercise using available geological, geophysical, geochemical, stable isotope and exploratory drilling data.. The simulation was carried out using the computer program MULKOM which is an integrated program computing two – phase flow in porous media and calculates mass and energy balance for each reservoir element providing output data of pressure, temperature, enthalpy and flow rates. The area around borehole 27 shows the region of maximum temperature of 1200 C at a depth of 350m in the southwestern part of the field with a geofluid discharge rate of 20 liters per second. Three simulation runs were carried out at a constant production rate of 05 lt/s, 10 lt/s and 20 lt/s for the power plant having 20 years of life span. The results indicate that the field can sustain continuous electric power generation of 0.3 MW for 20 years. The model calibrated as above was used to forecast the ultimate production from the reservoir and to identify the optimum development scenario.

Application of MH FE Model of Flow in Fractured Porous Medium on the Regional Scale

Authors: Klára Císařová, Jiřina Královcová, Jiří Maryška, Otto Severýn

The paper presents an application of our model for the simulation of underground processes. The model is based on the mixed-hybrid formulation. For its approximation are used the MH-FEM elements. The model enables to consider elements of different dimensions within one mesh (3D blocks, 2D planes, 1D lines), which allows to reflect different geological structures (porous media, fractures, fracture zones, intersections of large fractures, tubes, drill holes etc.) of considered rock massifs. The application is focused on the model of region of Cajamarca in Peru, where spa is located. The problem solved was to simulate an increse of pumping of mineral water and evaluate its consequences. The paper includes basis of the model, description of the selected region and mesh preparation. The results of the simulations are also included as well as the results of the sensitivity analysis.

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Aquifer structure identification and uncertainty evaluation using evolutionary stochastic inversion

Authors: Dylan R. Harp, Zhenxue Dai, Andrew V. Wolfsberg, Jasper A. Vrugt, Bruce A. Robinson, Velimir V. Vesselinov

Aquifer structure and facies hydraulic parameters are often large sources of uncertainty in flow and contaminant transport modeling. Typically, inverse modeling is performed assuming that the aquifer structure is fixed and performing the inversion solely on facies hydraulic parameters. Facies structures are often determined only based on borehole logs and indirect geophysical indicators of facies structure (gamma ray shaliness, electrical resistivity, etc.). A method derived in this study allows the coupling of aquifer structure identification and hydraulic parameter estimation utilizing an evolutionary stochastic inversion. Structure identification is performed by estimating the stochastic parameters of a transition probability model and updating the aquifer facies distributions with the indicator cokriging simulator. The stochastic property of these parameters requires a robust optimization algorithm capable of traversing the inherently complex objective-function space. The inversion utilizes a genetically-adaptive multimethod evolutionary search algorithm (AMALGAM-SO) to avoid local areas of attraction and identify optimal combinations of facies structure and hydraulic parameters. The method is illustrated by a synthetic problem used to test the methodology.

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Assessing the Hydrologic Impacts of Climate Change at the Watershed Scale

Authors: Martinus H. Brouwers, Jonathan F. Sykes, Stefano D. Normani

The increasing temperatures and changes to distributions of precipitation from climate change will intensify the hydrologic cycle which will directly impact surface water sources while the impacts to groundwater are reflected through changes in recharge to the water table. The Intergovernmental Panel on Climate Change reports that limited investigations have been conducted regarding the impacts of climate change on groundwater resources. This paper investigates the state of the science of conjunctive surface-subsurface water modeling with the aim of determining a suitable approach for conducting long-term transient simulations at the watershed scale. It is clear that while fully-integrated surface and ground water models are physically rigorous, they suffer in implementation from the often necessity to have a course discretization, particularly for the vadose zone, with this resulting in the inappropriate parameterization and use of Richards' Equation. Problems in the representation of overland flow are also apparent. These models typically have exceedingly long computational times that restrict the scale of their use and the obtained results are often not physically based but rather they are empirical and dependent on the discretization. As a result of our investigation, a combined or coupled modeling approach is adopted using HELP3 to simulate surface and vadose zone processes and HydroSphere to simulate saturated flow of groundwater. The methodology is applied to the Alder Creek Watershed near Kitchener-Waterloo, Ontario. The watershed is a suitable case study for the evaluation of climate change scenarios as it has been well characterized and it is relatively small in size. Input to HELP3 for the determination of spatially and temporally varying recharge at the water table include land use and land cover maps, soils maps and climate inputs of daily precipitation, temperature and solar radiation over a 40 year period. The distance between the ground surface and the water table is corrected from a first approximation using steady-state groundwater flow and recharge results. Though not as physically robust as the fully-integrated approach, the increase in computational efficiency gained by employing hydrologic models that more accurately describe the vadose zone processes allows for long-term simulations to be conducted at the watershed scale. Furthermore, relationships to approximate flow of water in porous media under freezing temperatures are built into the HELP3 model, allowing this coupled approach to conduct multi-year simulations. For the surface water system, the spatially varying conductivity values that control the flux between rivers and groundwater are determined using soil map data and a stream area that is related to the watershed contribution area. An optimization scheme is used to determine the elevation of stream bottoms. Two contrasting scenarios of climate change (i.e., drier and wetter futures) are evaluated relative to a reference scenario that is based on the historical 40 year climatic record of the region. The simulation results show a strong impact upon the timing of hydrologic processes, shifting the spring snow melt to earlier in the year leading to an overall decrease in runoff and increase in infiltration for both drier and wetter future climate scenarios. Both climate change scenarios showed a marked increase to overall evapotranspiration which is most pronounced in the summer months. The impacts to groundwater are more subdued relative to surface water. This is attributed to the climate forcing perturbations being attenuated by the shift of the spring snow melt and the transient storage effects of the vadose zone, which can be significant given the hummocky terrain of the region. The simulation results show a small overall rise of groundwater elevations resulting from the simulated increase in infiltration for both climate change scenarios.

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Assessing the Influence of Reservoir Operations Model Uncertainty for Comparative Studies Application

Authors: Levi Brekke, Nancy Parker, Tom Pruitt

Reclamation has explored the use of Monte Carlo analysis to reveal output uncertainties associated with the model structure and inputs of the Central Valley Project and State Water Project planning model, CALSIM II. This uncertainty analysis was applied to a single version of CALSIM II, where version is represented by water management scheme, system configuration, and/or level of land use development. In application, however, CALSIM II is typically used as a \"comparative\" analysis tool, where two versions of the model are run in parallel to reveal differences between alternative water management schemes, system configurations, or operations under different levels of land use development. The uncertainty about a single scenario condition does not reveal uncertainty about applying CALSIM II for comparative analysis. This work presents a method for doing the latter, featuring coordinated Monte Carlo analyses applied to two versions of CALSIM II, differing primarily by scenario land use (existing versus future). Each Monte Carlo realization reflects a potential collection of inputs within assumed limits of variation (i.e. water supply, demand, hydrologic, and environmental parameters) and is applied, as possible, to both CALSIM II study versions, differing by land use assumptions ("existing" versus "2030"). Uncertainty envelopes about each study version are then assessed, as is the uncertainty envelope about study differences measured as "future – existing" results specific to each realization of the coordinated Monte Carlo. Key challenges involved computational load and data handling across multiple applications in multiple formats, necessitating automation development (e.g., distributed computing, custom server-client software development). Presentation will highlight analytical and computational methods, as well as key results.

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Backward probabilities of groundwater contamination affected by subsurface heterogeneity and spatiotemporal nonlocal transport

Authors: Yong Zhang, Eric M. LaBolle

Backward probabilities of dissolved tracers, including the backward-in-time location and travel time probabilities, are used to evaluate the release history of contaminants, delineate well-head protection zones, calculate groundwater ages, assess aquifer vulnerability, identify sources of groundwater pollutants, and evaluate the influence of pumping on natural aquifer recharge. Backward probabilities are typically calculated by solving an adjoint (or backward in time) equation to the usual advection dispersion equation (ADE) [Neupauer and Wilson, 1999; 2001; 2003; 2004; 2007]. In this study, we extend Neupauer and Wilson's work by considering 1) the scale effect of backward probabilities in heterogeneous media, and 2) the influence of space and time nonlocalities on backward probabilities. The scale effect of backward probabilities of contamination was analyzed systematically for conservative tracers transport through regional-scale, heterogeneous media. Results show that the backward travel time and location probabilities are sensitive to the vertical size and location of screened intervals of capture wells. For example, in a typical alluvial aquifer system, the mean backward travel time can differ 20 years within a 2.5-meter-long screened interval, due to different flow paths reaching individual intervals under strong influence of subsurface hydrodynamics and heterogeneity. This behavior was expected from experience with the forward problem in heterogeneous systems. Thus the same challenges posed by the scale effect for the forward in time problem in heterogeneous media, including non-Fickian transport behavior at larger scales, also apply to the application of backward in time techniques. Contaminant transport through natural sediments is typically observed to be non-Fickian at all scales. Non-Fickian transport may be characterized by faster than linear growth of the centered second moment, or non-Gaussian leading or trailing edges (or tails) of a plume emanating from a point source. Numerical experiments indicate that realistic non-Fickian dispersion in locally heterogeneous environments cannot be captured by the traditional 2nd-order advection-dispersion equation (ADE) without extremely detailed (i.e., decimeter-scale) information of the connectivity of high and low hydraulic conductivity sediments. To investigate the backward probabilities of emerging non-Fickian representations of transport, we derived the backward equation corresponding to the space fractional ADE by extending Feller's [1971] integer-order adjoint method to the fractional order. The maximally skewed stable density in the forward equation was converted to its minimum counterpart, and the nonlinear Langevin equation was built to provide a fully Lagrangian simulator of the backward probabilities. We intend to derive the backward probabilities for the time nonlocal transport equation, so that the influence of multiple rate mass transfer between mobile and immobile zones on backward probabilities can be captured. Preliminary results demonstrate the influence of the heavy tails of the non-Fickian process on backward probabilities, an effect not captured with the usual adjoint of the 2nd-order ADE.

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Beyond the Black Box: Integrating Advanced Microbial Characterization Data with Subsurface Reactive Transport Models

Author: Timothy D. Scheibe, Pacific Northwest National Laboratory and Eoin L. Brodie, Lawrence Berkeley National Laboratory

Microbial processes are commonly represented in subsurface reactive transport models using relatively simple reaction-rate models that do not account for complexities of microbial function and community dynamics. While this approach has been effective in many settings, we believe there is now an opportunity to significantly improve the foundational basis of reactive transport model predictions by integrating newly available microbial characterization data and understanding. The field of environmental microbiology has recently taken a quantum leap due to developments in molecular biology, enabling holistic views of complex microbial communities. Recent technological advances such as high-throughput multiplex sequencing, high-density microarrays, and environmental proteomics now provide a deluge of information on the nature and function of microbial communities. This session will explore novel approaches to incorporating this information into predictive simulations of biogeochemical processes having relevance to scientific and engineering problems. Such approaches include direct linkage of genomics-based models of cell function (in silico models) and reactive transport codes, and modeling of environmental-microbial interactions using approaches such as logical networks, boosting, and random forests.

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Calibration of the NCAR Community Land Model (CLM) using GRACE and Baseflow

Authors: Min-Hui Lo, James Famiglietti

Several recent studies have shown the significance of representing groundwater in land surface hydrologic simulations. However, optimal methods for model parameter calibration in order to realistically simulate baseflow, water storage, and groundwater depth have received little attention. Most studies still use globally constant groundwater parameters due to the lack of available datasets for calibration. Moreover, when models are calibrated, various parameter combinations are found to exhibit equifinality in simulated total runoff due to model parameter interactions. In this study, a simple lumped groundwater model is incorporated into the Community Land Model (CLM), in which the water table is interactively coupled to soil moisture through the groundwater recharge fluxes. The coupled model (CLMGW) is successfully validated in Illinois using a 22-year (1984-2005) monthly observational dataset. Total water storage changes from GRACE and baseflow estimates from the digital recursive filter technique are used to calibrate the CLMGW parameters. Using the optimal parameter sets identified from GRACE and baseflow calibrations, flow partitioning, total water storage changes, and water table depth simulations using CLMGW are improved, and the equifinality problem is alleviated. For other regions that lack observations of water table depth, the multi-objective calibration approach can be used to enhance parameter estimation and constrain water storage and its partitioning simulations. The calibrated CLMGW is applied to the entire US to study the impact of groundwater on land hydrologic memory.

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Carbon and Water Management in the Context of ECBM

Authors: Wenjuan Lin, Marjan Jamshidi, Kristian Jessen, Anthony Kovscek

Geological sequestration of carbon dioxide, coalbed methane production, and water resources are linked. Enhanced coalbed methane (ECBM) recovery by injection of CO2 or by injection of mixtures of CO2 and N2 recovers additional natural gas resources while at the same time sequestering CO2 in the subsurface. The dynamics of ECBM recovery processes are determined in large part by the sorption behavior of mixtures of CH4, CO2 and N2 on the coal surface. Coalbeds are typically saturated with water and sometimes in hydraulic communication with an aquifer. The traditional approach for producing CBM relies on a reduction of the gas partial pressure in the coal seam by pumping formation water to the surface. Disposal of the produced water may pose an environmental challenge as harmful impurities must be removed. In addition to the potential of storing significant amounts of CO2, ECBM processes may also help in reducing the amounts of formation water that is co-produced with the natural gas. Conventional simulation tools use the extended Langmuir model for predicting the sorption behavior of the gas mixtures that form during a displacement process. In previous work, we demonstrated the accuracy of this approach for binary CH4/CO2 and CH4/N2 displacements by comparison to lab scale experiments. The extended Langmuir model was unable to describe the behavior of ternary CH4/CO2/N2 displacements. Adsorption hysteresis is a complicating factor also. This paper investigates the accuracy of ternary gas displacement calculations relative to experimental observations. We demonstrate that sorption models more sophisticated than the extended Langmuir model are needed to represent the dynamics of these multicomponent, multiphase systems accurately. We present a comparison of displacement calculations using the Ideal Adsorbate Solution model (IAS) relative to the behavior predicted from standard calculations in terms of the timing and amounts of produced gas and water. We conclude the paper by discussing the current challenges related to modeling and simulation of ECBM production in concert with CO2 sequestration and conservation of water resources.

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Climate Change and Water Resources: Tools for Assessments and Planning

Author: Michael Dettinger, US Geological Survey, Scripps Institution of Oceanography, La Jolla, CA

Climate change has the potential to disrupt water resource systems by changing the timing, amounts, and quality of water supplies, and by changing flood and drought characteristics, consumptive and transmission losses, and water demands from their historical norms in as-yet unpredictable ways. Many agencies are mobilizing to assess water-resource vulnerabilities and to incorporate climate change in planning and decision making. These efforts, however, are uncovering a number of difficult methodological and computational challenges, including needs to:

- Identify key and most credible climatic changes in climate projections and then project those changes down to hydrologically relevant scales for resource modeling and other uses (credible projection and downscaling)
- Recognize and distinguish between natural and human-induced hydrologically relevant hydroclimatic changes through detailed comparisons of observations and simulations (detection and attribution)
- Improve the observational basis and modeling representations of relevant climatic influences in water-resources models and computations (observations and climatic linkages)
- Model and incorporate climate-change probabilities and risks for decision making (probabilistic methods)
- Sort through and distinguish between differing management responses (feasibility and optimization methods)

These challenges are often aggravated by the large dimensions of data fields, models, and feasibility spaces, and the limited numbers of available projections, process models, observations, and relevant historical examples. This session solicits research contributions that address these needs through theoretical advances and practical applications. We encourage presentation of examples of innovative solutions for real-world water-resource systems with prospects for widespread applicability.

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Climate change impact on hydrological extremes in Belgium

Authors: Boukhris Omar el Farouk, Patrick Willems

A methodology to analyzes potential climate change impacts on hydrological extremes along rivers in Flanders (Belgium) has been developed. The resullts show that hydrological modelling techniques driven by climate modelling techniques and climate change scenarios enable a prediction of the long-term evolution of the hydrological system of the studied area. The climate change impact analysis is based on a continious simulation approach: The hydrological system behaviour of the main rivers in the Scheldt River Basin District is modeled for an observed historical period and for a future change from the control period (1961-1990) to the predicted period (2071-2100) under forcing of a modified (predicted) climate. The climate change impact on hydrological extremes is assessed through the comparison of key variables of the hydrological system for the two periods (e.g., runoff peaks, low flow values, overland flow and potential evapo(transpi)ration). The overall modelling procedure is completed through a set of 24 climate model simulations highly resolute (derived from the PRUDENCE climate project), local scale lumped conceptual hydrological models (NAM of DHI), hydrodynamic models (MIKE11 of DHI) and models for topographical information (DEM: Digital Elevation Models) and risk calculation models covering the studied area. An appropriate downscaling method has been developed counting for variable statistical properties as intensity and frequency. This method lead to created potential climate change scenarios for Flanders based on sequences of low, mean and high variation factors of the variables of precipitation and potential evapo(transpi)ration. The modelling procedure results state that the predicted climate evolution induces a significant reduction of the low flows due to a considerable hydrological regime modification. As for high flows (flood risk), the results range from increasing to decreasing depending on the climate change scenario and thus counting for a large uncertainty. Overland flow follows similar patterns as for the high flows while evapo(transpi)ration shows systematic increase as a result of regional warming. A statistical method has been implemented for the quantification of the modelling uncertainties induced by the created climate change scenarios and by natural variability. It is based on ensemble modelling of the regional climate model simulations and on Monte Carlo simulations to account for the effect of uncertainties in the selected climate change scenarios due to natural variability when comparing the climate model results with historical data.

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Climate Change Impacts on Crop Water Requirements, Soil and Ground Water Salinity in California's San Joaquin Valley

Authors: Jan W Hopmans, Gerrit Schoups, Ed Maurer

Climate change in the western US is predicted to produce significant changes in temperature, precipitation amount and their spatial/temporal distributions. These changes will have profound affects on California's water resources and on both natural and agricultural ecosystems. California, with its limited water supply and the reliance of the State's economy on agriculture, faces enormous challenges in the near future, to analyze and to forecast climate change impacts. A recent series of white papers (California Climate Center, 2005) laid out the impacts of possible climate change scenarios in California resulting from increasing atmospheric concentration of green house gases (GHGs) on coastal sea level, precipitation, water resources, agriculture, public health, forestry, and electricity production and demand. Results were based on three GHG scenarios: lower emission, medium-high emission, and higher emission scenarios, using 3 different Global Climate Models (GCM's). California's farmers are expected to respond to reducing surface water supplies and/or increasing irrigation water requirements by supplementing available irrigation waters by increased groundwater pumping. However, increased pumping will increase energy costs as hydraulic heads in the aquifers drop, whereas the lesser quality of groundwater will generally increase soil salinity. The results of a recently developed hydrosalinity model will be presented, summarizing impacts of climate change on irrigation water availability, crop water requirement (ET) and soil salinity for a 1,400 km2 irrigated area in the San Joaquin Valley that includes a large part of Westlands Water District (WWD), Broadview Water District (BWD) and 11 additional water districts. This model couples subsurface hydrology with climate change and will provide for an integrated approach towards understanding the impact of climate change on CA's irrigated agriculture, including the forecasting of the effect of various climate change scenarios on potential crop ET for typical crops in the SJV; and the impact of climate change on irrigation water availability, crop water requirement and soil salinity in the 21st century.

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CO2 Sequestration

Author: Hamdi Tchelepi, Stanford University

Numerical simulation is expected to play an important role in the planning, development, and monitoring of practical subsurface CO2 sequestration projects. Several important challenges must be met before a simulation-based approach can be used with confidence. Here, we solicit papers that describe experimental and numerical approaches for exploring the multiscale physics associated with subsurface CO2 sequestration processes, from the pore scale to the field, with emphasis on physically based models that bridge the scales in a coherent and consistent mathematical and numerical framework. This includes areas related to (1) static and dynamic data integration of highly detailed models, (2) quantification of prediction uncertainty due to missing information, (3) small and large-scale experiments targeted at the CO2-brine system, (4) multiscale numerical formulations suited for accurate modeling of the post-injection period, where buoyancy, diffusion, and dissolution are the dominant mechanics for flow and transport.

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Comparative Inverse Modeling With Combination of Multiphysics Codes and Parameter Estimation Snap-on Tools

Authors: Hanieh Haeri, Laura Foglia, Timothy Ginn

Inverse problems in hydrology and hydrogeology are challenging due to non-uniqueness. One avenue to reduction of non-uniqueness involves use of multiple data sets governed by the same aquifer property to be estimated, such as piezometric head and groundwater age. Since head information is governed by a diffusion equation and age information governed by an advection-dispersion-reaction equation, their coupling may sharpen inverse problem solutions. We apply multiphysics modeling of simplified, idealized problem in the forward sense to solve simultaneously the steady-state flow and mean age equations, the output of which is used as input to an indirect inversion scheme (UCODE_2005) to calibrate some of the parameters involved. The flow domain is a drawn from a classical two-dimensional problem with three of four boundaries corresponding to no-flow conditions, and the forward simulation includes a convergence analysis of grid resolution to address accuracy. The inverse calibration includes sensitivity analysis via composite scaled sensitivity (CSS), dimensionless scaled sensitivity (DSS), and parameter correlation coefficient (pcc). In the inverse part, we investigate the role of sample data location on the non uniqueness problem. We demonstrate nonuniqueness of the inverse for several different hypothesized sets of calibration data, including noise vs. no-noise cases, dense vs. sparse sampling of head and age, and nonuniform sampling densities. We explore the reduction in non-uniqueness per additional sampling location in order to identify most valuable locations for additional sampling.

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Comparison of Laplace Approximation and Monte Carlo Methods for Bayesian Model Selection and Multimodel Averaging

Authors: Ming Ye, Dan Lu

Hydrologic systems are open and complex, rendering them prone to multiple conceptualizations and mathematical descriptions. There has been a growing tendency to postulate several alternative hydrologic models for a site and use model selection criteria to (a) rank these models, (b) eliminate some of them and/or (c) weigh and average predictions and statistics generated by multiple models. While there are several model selection criteria (e.g., AIC, AICc, BIC, and KIC), this study is focused on the Bayesian criteria of BIC and KIC, two asymptotic Laplace approximations of model likelihood function in the framework of Bayesian model averaging. KIC is theoretically close to BIC when a large amount of data is used to estimate model parameters and evaluate the two criteria. This, however, has not been investigated for hydrological models. While KIC is more accurate than BIC when the sample size is small, estimating KIC is hampered by evaluating the observed Fisher information matrix (or the Hessian matrix). In this study, we use Monte Carlo method to estimate the model likelihood function, and the result is used as a "yardstick" to evaluate the two criteria. Our numerical example is based on alternative geostatistical models whose function forms are known. This makes it possible to derive analytical form of the Fisher information matrix. In addition to the analytical solution, we also evaluate its expected value with respect to the data. The expected value is about 10% smaller than the analytical value, but its corresponding model likelihood function is about two times larger than the Monte Carlo result. The difference is also related to the model parameter estimates. The study demonstrates importance of the observed Fisher information matrix on the model selection. It is recommended to use KIC rather than BIC for model selection and model averaging.

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Compensated Root Water and Nutrient Uptake

Authors: Jiri Simunek, Jan W. Hopmans

Plant root water and nutrient uptake is one of the most important processes in subsurface unsaturated flow and transport modeling, as root uptake controls actual plant evapotranspiration, water recharge and nutrient leaching to the groundwater, and exerts a major influence on predictions of global climate models. In general, unsaturated models describe root uptake relatively simple. For example, root water uptake is mostly uncompensated and nutrient uptake is simulated assuming that all uptake is passive, through the water uptake pathway only. We present a new compensated root water and nutrient uptake model, implemented in HYDRUS. The so-called root adaptability factor represents a threshold value above which reduced root water or nutrient uptake in water- or nutrient-stressed parts of the root zone is fully compensated for by increased uptake in other soil regions that are less stressed. Using a critical value of the water stress index, water uptake compensation is proportional to the water stress response function. Total root nutrient uptake is determined from the total of active and passive nutrient uptake. The partitioning between passive and active uptake is controlled by the a priori defined concentration value cmax. Passive nutrient uptake is simulated by multiplying root water uptake with the dissolved nutrient concentration, for soil solution concentration values below cmax. Passive nutrient uptake is thus zero when cmax is equal to zero. As the active nutrient uptake is obtained from the difference between plant nutrient demand and passive nutrient uptake (using Michaelis-Menten kinetics), the presented model thus implies that reduced passive nutrient uptake is compensated for by active nutrient uptake. In addition, the proposed root uptake model includes compensation for active nutrient uptake, in a similar way as used for root water uptake. The proposed root water and nutrient uptake model is demonstrated by several hypothetical examples, for plants supplied by water due to capillary rise from groundwater and surface drip irrigation.

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Component Additivity Approach for Uranium Retardation in Sandstone Host Rocks

Authors: Anke Richter, Cordula Nebelung, Vinzenz Brendler

Sandstone is one of the most important host rocks for uranium ore deposits, e.g. in Germany (Koenigstein) or the Czech Republic (Pribram). Any remediation efforts of respective mining legacies thus require a detailed understanding of this system. Namely the sorption in this complex rock is not fully understood. One widely accepted approach (Component Additivity – CA, cf. [1]) to describe the sorption is based on the assumption that the surface of a complex mineral assemblage is composed of a mixture of severe phases whose surface properties are known from independent studies. An internally consistent SCM (surface complexation model) database can be developed that describes the adsorption reactions of solutes to each phase. The fitting of data of the complex system is not necessary, provided sufficient information on component phases is available. We predicted the sorption of uranium(VI) on sandstone using the results of the surface characterization of the assemblage and published data for adsorption onto the pure mineral constituents. The results were compared with batch sorption experiments using natural and synthetic sandstone (mixture of the main components quartz, muscovite, and hematite). The sorption of U(VI) on natural and two synthetic sandstone (I and II) was investigated in batch sorption experiments (air atmosphere, 12.5 g/L, 0.1 M $NaClO_4$, pH dependence (pH: 3-11 at [U(VI]=1E-6 M), and uranium concentration dependence ([U(VI)]: 1E-9 - 1E-3 M at pH 5)). We had to consider the natural uranium concentration dissolved from the sandstone at low concentrations. The synthetic sandstone was a mixture of quartz with muscovite and hematite. The pH dependence shows a sorption peak between pH 6 and 7. In the experiments with varying uranium concentrations, the sorption ranges from 95% (1E-9 M) to 7% (1E-4 M) on natural sandstone, and from 80% (1E-9 M) and 2% (1E-4 M) on synthetic sandstone. The modeling of U(VI) sorption on sandstone was performed using the CA approach. We assumed just one type of surface sites on each mineral and applied a model with simple electrostatics, the Diffuse Double Layer Model (DDLM). For the modeling the code MINTEQA2 (Version 4.03, US EPA, May 2006) was used. The aqueous species were taken from the NEA-TDB [2]. As surface reactions we considered the protolysis of quartz, hematite, muscovite, the U(VI) surface complexes of quartz, hematite, muscovite (monomer, dimer) and the ternary U(VI) surface complexes of quartz and hematite with carbonate. The contribution of each mineral to the total surface area of the mixed phase was calculated according to its proportion (by weight). Fig. 1 shows the model predictions of the pH dependence of the U(VI) sorption on natural and synthetic sandstone I compared to the experimental results. Despite of a slight shift of the predicted curve to lower pH in both systems, a good accordance with experimental values were found. Obviously, the sorption is strongly influenced by the small amount (0.5 %) of hematite. For the experiments at higher U(VI) initial concentration, a precipitation of schoepite was predicted. This precipitation we found experimentally for the synthetic sandstone at 1E-3 M U(VI). As schoepite is an aged mineral, it is unlikely to be formed within the experimental duration of five days. A subsequent exclusion from the list of allowed phases led to a predicted precipitation of both soddyite and metaschoepite. Acknowledgement Funding by the BMBF (02C1144) is gratefully acknowledged. References [1] Davis, J.A. et al. (1998) Application of the surface complexation concept to complex mineral assemblages. Environ. Sci. Technol. 32, 2820-2828. [2] Guillaumont, R. et al. (2003) Update on the chemical thermodynamics of U, Np, Pu, Am, Tc. Elsevier, Amsterdam.

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Computational efficiency of contaminant transport modeling using the Analytic Element Method in combination with the deterministic Streamline Method

Authors: Karl W. Bandilla, Igor Janković, Alan J. Rabideau

Computational limitations continue to constrain the scale of supra-regional scale ground water models. A recent approach to increase the possible domain size is to use a combination of the Analytic Element Method (AEM) and the deterministic Streamline Method. AEM is used to solve the flow problem and the deterministic Streamline Method is used for contaminant transport modeling. AEM is an alternative to the Finite Element (FEM) and Finite Difference Methods (FDM) for solving subsurface flow problems on large scales. The domain is discretized along the hydrogeologic elements (e.g. surface water features, zones where conductivity differs from the surrounding conductivity, wells, etc.) instead of using a grid discretization as in FEM and FDM. Two features that make AEM well suited for a basis of the Streamline Method are particle tracking without interpolation due to the representation of the entire flow field instead of nodal values, and the strong parallel processing capabilities. In the implementation presented here a 2D vertically averaged steady-state groundwater flow simulator is used to solve the flow problem. Vertical velocities are computed based on mass balance considerations, thus leading to a quasi 3D flow field. The 3D particle tracks can then be used in the Streamline Method for contaminant transport. The Streamline Method discretizes the transport domain by converting curvy 3D streamlines into straight 1D streamlines. The conversion is achieved by transforming the Cartesian coordinates of the transport domain into a 1D coordinate system based on the "time-of-flight" coordinate, which describes the time for a particle to travel the distance along the streamline. The transport along the streamline is then solved using FEM or FDM. Two beneficial features of the Streamline Method are the comparative ease of solving a set of uncoupled 1D models, instead of a single fully-coupled 3D model, and the independence of streamlines which leads to efficient parallel processing. It has been shown, that this approach allows to model flow and reactive transport in a 900 sqkm domain, while preserving stream level details. This work examines several aspects of the new AEM/Streamline approach, including parallel processing performance and streamline velocity averaging techniques. It can be shown, that the parallel performance strongly depends on load balancing. Therefore, two load balancing schemes are explored. One scheme distributes streamlines based on the number of streamlines in the domain (i.e., each processor computes about the same number of streamlines), while for the other scheme distributes streamlines "on the fly" (i.e., processors are given a new streamline once they finish computing the current streamline). In an attempt to better represent the influence of inhomogeneities in hydraulic conductivity a new approach for velocity averaging will be demonstrated. In this approach velocities at the stream tube boundary are incorporated into the average velocity, instead of just using the velocities along the streamline. The goal of this approach is to reduce the number of streamlines, and thus increase computational efficiency.

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Computational Environments for Coupling Multiphase Flow, Transport, and Mechanics in Porous Media for Modeling Carbon Sequestration

Author: Mary F. Wheeler, Center for Subsurface Modeling, , Institute for Computational Engineering and Sciences, The University of Texas at Austin

There is consensus in the scientific community that increased levels of greenhouse gases contribute to recent trends in global warming and dramatic changes in weather patterns. Geologic sequestration by injection of CO2 into deep brine aquifers and reservoirs represents one of the most promising approaches for reducing atmospheric CO2. The basis for this potential is the huge global storage capacity existing in geologic formations (primarily deep saline aquifers) and the availability and close proximity of potential injection sites to power generation plants. However, such injections pose significant technical issues in efforts to ensure safety, to minimize leakage probability on a time scale of hundreds or even thousands of years, and to gain public acceptance.

A key goal of our work is to produce a prototypical computational system to accurately predict the fate of injected CO2 in conditions governed by multiphase flow, rock mechanics, multi-component transport, thermodynamic phase behavior, chemical reactions within both the fluid and the rock, and the coupling of all these phenomena over multiple time and spatial scales. Even small leakage rates over long periods of time can unravel the positive effects of sequestration. This effort requires high accuracy in the physical models and their corresponding numerical approximations. For example, an error of one percent per year in a simulation may be of little concern when dealing with CO2 oil recovery flooding, but such an inaccuracy for sequestration will lead to significantly misleading results that could fail to produce any long-term predictive capability. It is important to note that very few parallel commercial and/or research software tools exist for simulating complex processes such as coupled multiphase flow with chemical transport and geomechanics.

In order to address this challenge a robust reservoir simulator comprised of coupled programs that together account for multicomponent, multiscale, multiphase flow and transport through porous media and through wells and that incorporate uncertainty and include robust solvers is required. The coupled programs must be able to treat different physical processes occurring simultaneously in different parts of the domain, and for computational accuracy and efficiency, should also accommodate multiple numerical schemes. In addition, this problem solving environment or framework must have parameter estimation and optimal control capabilities. We present a "wish list" for simulator capabilities as well as describe the methodology employed in the IPARS software being developed at The University of Texas at Austin.

Tuesday's At-A-Glance

Computational improvements for coupled 3D soil-root flow models

Authors: T. Schröder, M. Javaux, J. Vanderborght, B. Körfgen, H. Vereecken

Three dimensional models based on water potential differences and hydraulic conductivities between soil and root are nowadays needed to asses spatial and temporal variability of water flow and solute transport and the uptake of water by plant roots. Recently, improvements are made in such 3D models to describe local root water uptake at the interface between soil and root. Further improvements are needed with respect to computational times. The need to model water flow in soils with large root structures increases. Mainly due to advances in experimental techniques. We can measure with higher accuracy and soon we will be able to quantify larger root structures at the plant scale. With increasing root structures the degrees of freedom in the models will increase. Effective mathematical techniques need to be applied to speed up the process of solving the soil and root system and to simulate accurate results. Currently, the soil and root system are solved as coupled systems, whereas it would be quicker if we are able to solve them at once. We also have the possibility to use supercomputers, with multiple processors, to solve our system parallel. Furthermore, the usage of adaptive or parallel adaptive grids is needed to gain accuracy and decrease the computational time. The current developments and possibilities using the 3D soil-root flow model R-SWMS will be discussed.

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Computational Intelligence Runoff Modeling by Means of Multi-agent Systems

Authors: Roman Neruda

Hybrid models, including combinations of computational intelligence methods such as neural networks, genetic algorithms and fuzzy logic controllers, seem to be a promising and extensively studied research area [1]. We have designed a distributed multi-agent system [2] that provides a support for an easy creation of hybrid AI models by means of autonomous software agents [3]. Autonomous agents are small self-contained programs that can solve simple problems in a well-defined domain. In order to solve complex problems, agents have to collaborate, forming Multi-Agent Systems (MAS) that in our case represent the hybrid computational intelligence models. A key issue in MAS research is how to generate MAS configurations that solve a given problem. In most systems, an intelligent (human) user is required to set up the system configuration. Developing algorithms for automatic configuration of Multi-Agent Systems is a major challenge for AI research. We present results of a small test-case a rainfall-runoff modeling by means of multi-layer perceptron networks (MLP) and radial basis (local units) networks (RBF) [4]. The Ploucnice river in North Bohemia has been chosen as an experimental catchment to calibrate and evaluate the models [5]. It has its origin in the altitude 654m upon sea level, and it flows to Elbe River in Desna town in 122m upon sea level. The considered catchment area is 268sq.km (out of 1193 sq.km in total), the flow length is 106km. Historical daily flow and rainfall data has been split into training data - 1000 days between Jan 1999 and Sep 2001, and testing data - between Oct 2001 and Apr 2003. Training data are used to set the network parameters during the training process, while the testing batch is used to verify the network ability to model previously unseen data. Series of experiments have been performed, comparing MLP and RBF networks with different topologies trained by several algorithms combining back propagation with momentum term, clustering, pseudo-inverse matrix, regularization (with suitable regularization parameters found by cross-validation) and genetic algorithms. The benefits of MAS realization of the computational intelligence models is in the semi-automated way of changing the components (neural networks, learning algorithms) and distributed execution over a cluster of Linux workstations. The best results were achieved by the 2-5-7-9-1 percpetron network trained with the back propagation algorithm with momentum term. Also, perceptron networks in general achieved better results with less parameters than RBF networks. We believe that this is because networks with more free parameters tend to be over-trained more easily, thus achieving better training error, but worse testing error. For further experiments we would like to test models based on two days advance forecast, and consider finer hourly scale of the data. In cooperation with the Czech Hydro-meteorological Institute we plan to deploy the model on-line and combine it with the precipitation forecasts. In its final stage, the fine-tuned system should help to forecast extreme runoff values, and help in the early flood danger detection. [1] P. Bonissone. Soft computing: the convergence of emerging reasoning technologies. Soft Computing, 1:6–18, 1997. [2] G. Beuster, R. Neruda, P. Krusina, and P. Rydvan. Towards building computational agents schemes. In Artificial Neural Nets and Genetic Algorithms. Proc. of the ICANNGA 2003 Conf., 2003. Springer-Verlag. [3] G. Weiss, editor. Multiagent Systems. The MIT Press, 1999. [4] R. Neruda, P. Kudova, Learning Methods for Radial Basis Functions Networks. Future Generation Computer Systems, 2005, 21, 1131-1142. [5] M. Neruda, R. Neruda; P. Kudova. Forecasting Runoff with Artificial Neural Networks. In Progress in Surface and Subsurface Water Studies at Plot and Small Basin Scale. Paris : UNESCO, 2005. 65-69.

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Computer simulation of coupled flow and mineral precipitation/dissolution in porous media: A level set approach

Authors: Hai Huang, Paul Meakin, Xiaoyi Li

The nonlinear coupling of fluid flow, reactive chemical transport and pore structure changes due to mineral precipitation (or dissolution) in porous media play a key role in a wide variety of processes of scientific interest and practical importance. Significant examples include the evolution of fracture apertures in the subsurface, acid fracturing stimulation for enhanced oil recovery and immobilizations of radionuclides and heavy metals in contaminated groundwater. We have developed a pore-scale simulation technique based on level set interface tracking method for modeling coupled reactive flow and structure evolution in porous media and fracture apertures. Advection, diffusion, and mineral precipitation resulting in changes in pore geometries are treated simultaneously by solving fully coupled fluid flow and reactive solute transport equations. In this model, the reaction-induced evolution of solid grain surfaces is captured using a level set method. A sub-grid representation of the interface, based on the level set approach, is used instead of a pixel representation of the interface often used in cellular-automata and most lattice-Boltzmann methods. The model is validated against analytical solutions for simplified geometries. Precipitation processes were simulated under various flow conditions and reaction rates, and the resulting pore geometry changes are discussed. Quantitative relationships between permeability and porosity under various flow conditions and reaction rates are also reported.

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Computer simulations of multiphase fluid motion in unsaturated fracture apertures and porous media: A volume of fluid (VOF) approach

Authors: Hai Huang, Paul Meakin

We successfully applied a popular multiphase flow simulation method in computational fluid dynamics, the volume of fluid (VOF) method, to model the liquid motion in partially saturated fracture apertures and fracture network under a variety of flow conditions. The effects of inertial forces, viscosity, gravity acting on the fluid densities, fracture wall wetting dynamics, and the pressure drop across the fluid-fluid interfaces due to surface tension are systematically incorporated into the model. The models has a Navier-Stokes equation solver coupled with an interface tracking method that is capable of handling large topological changes of the interfaces without resorting to dynamic mesh refinement. Complex dynamics of fluid-fluid interfaces and free surfaces in fracture apertures and pore spaces are handled very well by this model. The new simulation technique provides quantitative ways for better understandings of the fundamental physics governing unsaturated fluid motion in fractures and porous medium. Our simulation results reveal that fluid motion in unsaturated fractures is complex, even for very simple fracture geometries under constant liquid injection conditions. Different flow behaviors within unsaturated fractures, including continuous film flow, intermittent mixed film flow, stationary capillary droplet formation and snap-off/reconnection, can coexist, depending on the fracture geometry, wetting behavior, fluid properties and so on.

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Continuous Time Random Walk Analysis of Solute Transport in Fractured Porous Media

Authors: Jens Birkholzer , Andrea Cortis

The objective of this work is to discuss solute transport phenomena in fractured porous media, where the macroscopic transport of contaminants in the highly permeable inter-connected fractures can be strongly affected by solute exchange with the porous rock matrix. We are interested in a wide range of rock types, with matrix hydraulic conductivities varying from almost impermeable (e.g., granites) to somewhat permeable (e.g., porous sandstones). In the first case, molecular diffusion is the only transport process causing the transfer of contaminants between the fractures and the matrix blocks. In the second case, additional solute transfer occurs as a result of a combination of advective and dispersive transport mechanisms, with considerable impact on the macroscopic transport behavior. We start our study by conducting numerical tracer experiments employing a discrete (microscopic) representation of fractures and matrix. Using the discrete simulations as a surrogate for the "correct" transport behavior, we then evaluate the accuracy of macroscopic (continuum) approaches in comparison with the discrete results. However, instead of using dual-continuum models, which are quite often used to account for this type of heterogeneity, we develop a macroscopic model based on the Continuous Time Random Walk (CTRW) framework, which characterizes the interaction between the fractured and porous rock domains by using a probability distribution function of residence times. A parametric study of how CTRW parameters evolve is presented, describing transport as a function of the hydraulic conductivity ratio between fractured and porous domains.

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Continuum Darcy approach for surface-subsurface flow and transport modelling : application to the Thies plot experiment in Senegal

Authors: WEILL S., MOUCHE E., PATIN J., MUGLER C.

A new approach modeling surface/subsurface flow and transport in a continuous way is presented. Darcy, Richards and diffusive wave equations are used respectively to describe variably saturated and surface flows. Diffusive wave equation is turned into a non-linear Darcy equation, which looks like Richards one. Runoff is then assimilated as flow in a porous medium having special properties. A gridded layer of this particular porous medium is introduced in the computational domain at the top of the physical land surface. Its water content and hydraulic conductivity functions are then defined to simulate correctly overland flow. Using this runoff layer concept, the whole surface/subsurface flow dynamics is described in a unified manner by a single Darcy type equation in a porous continuum that extends from subsurface to land surface. Pressure and fluxes are continuous through land surface. Tracer transport in the whole domain is described by an advective-dispersive equation. Once again, using the runoff layer concept, transport is described in a unified manner in the surface/subsurface Darcy continuum. This modelling approach is implemented in a finite element code called Cast3m. The plot scale experiment realized at Thies, Senegal, is then presented. The rainfall-simulation experiments were designed by the IRD (Research and Development Institute) to study runoff generation processes. Different velocity fields measurements and tracer experiments (mainly salt injections in surface water) were performed on this 10m x 4m plot. The dominant runoff generation process is Hortonian runoff. Two experiments were reproduced with the model presented in the first part. In the first modelling exercise, measured and simulated surface velocity fields are compared, allowing to verify the implemented surface model and to study the influence of rugosity on runoff velocity fields. The second modelling exercise deals with transport and dispersion at the plot scale. Salt injections on land surface during runoff are simulated, and measured and simulated tracer breakthrough curves are compared and their scale dependency is discussed . Partitioning between infiltration and overland flow is also considered. First results are encouraging and allow to think that the developed Darcy continuum model will be a useful tool to study runoff generation processes and tracer transport at the plot scale.

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Cost-economical Optimization and Feasibility Investigation of Groundwater Management Schemes for Groundwater Flow

Authors: P. Arlai, M. Koch

Even though the simultaneously acting two cradles of the major saline pollution in the Bangkok aquifer system have already been clarified by the authors (Arlai et al., 2006a;b), namely, (1) vertical seepage of saline water from marine clay layers and, (2) horizontal sea water intrusion from the Gulf of Thailand and some sustainable aquifer remediation concepts, consisting in both non-constructive and integrating policies & constructive measures have subsequently been proposed (Arlai et al., 2007), the latter may globally not be optimal, neither in terms of hydraulics nor of economics, as they have exclusively been determined by human judgment, or so-called "trial & error". Furthermore, the numerical method used there, i.e. MODFLOW-96&MT3DMS, did not yet take into account the density-dependent effects of the saline concentrations on the flow and solute transport. In the present contribution we will overcome these two limitations partly by a) application of the groundwater management optimization module GWM, embedded in MODFLOW-2000, to further optimize hydraulically and economically the number of recharge-,clean-up wells and three new water trade-off concepts for the given set of head targets. In addition to an earlier study, three new schemes that use a "water supply trade-off concept" for the in-lieu water supply are optimized under hydraulic as well as economical considerations. b) use of the variable-density model SEAWAT-2000 to investigate the density effects on the optimized schemes proposed in a) and on the non-constructive schemes proposed earlier. Based on the results of a) and b) a careful evaluation and comparison of the hydraulic- and of the groundwater-quality efficiency of the optimal schemes is performed, taking into the consideration the total financial costs of all schemes investigated. Eventually one feasible management scheme is proposed for realization to local water authorities that may help to revert the precarious groundwater situation of this indispensable groundwater resource of Thailand in the future. References: Arlai, P., M. Koch., S. Koontanakulvong and Weerapol B. (2006a), Numerical Modeling as a Tool to Investigate the Feasibility of Artificial Recharge to Prevent Possible Saltwater Intrusion into the Bangkok Coastal Aquifers System, Proceedings of "Groundwater Hydraulics in Complex Environments", Toulouse, France, 12-14 June, 2006. Arlai, P., M. Koch and S. Koontanakulvong, Numerical (2006b), Investigation of the Cradle of Saline Contamination and Effective Remediation Schemes for Amending Saline Water Pollution Problem in the Bangkok Coastal Aquifers System , 3rd APHW Conference , Bangkok, October 16-18, 2006, Poster. Arlai, P., M. Koch and S. Koontanakulvong (2007), Embedding an Optimization Module within a 3D Density Dependent Groundwater and Solute Transport Model to determine an effective Groundwater Management Scheme in the Bangkok Aquifers System, Asian Simulation Modeling 2007, Chaing Mai, Thailand, January 9-11, 2007.

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Coupled Numerical Simulation of Shallow Geothermal Energy Systems

Authors: Prof. Dr.-Ing. Rolf Katzenbach, Dipl.-Ing. Frithjof Clauss, Dipl.-Ing. Thomas Waberseck, Dipl.-Ing. Isabel Wagner

The rapid growth of cities and metropoles and the increasing demands in living comfort in many regions cause a rising energy demand for building tempering. Therefore economically efficient and technically reliable energy sources are needed. The geothermal use of subsoil can be a solution, since it reduces the use of fossil fuels tremendously, which are limited in their availability, and thereby also sustains the reduction of CO2 emissions and other greenhouse gases. Geothermal Energy is absolutely renewable and sustainable. Various technical solutions for the thermal use of subsoil such as ground source heat pumps, borehole heat exchangers, energy piles and others are available. These geothermal facilities require a well-engineered dimensioning and design accounting for the complex influencing quantities and basic conditions in order archive efficient and economic systems. Generally, the use of geothermal energy gives rise to legal questions as the thermal influence of a geothermal system on the surrounding subsoil could affect neighboring premises. Comprehensive simulations can give investors the desired reliability and legal certainty. Therefore, a proper modeling of the heterogeneous multi-phase medium subsoil with its complex flow and heat transport properties is of significant importance. Depending on the soil and groundwater conditions of a specific site, different mechanisms dominate the heat transport in the influenced subsoil region. Because of the complexity analytical methods are not sufficient to model the real thermal behavior properly. Only coupled numerical simulations can consider the transient flow and heat transport situation, the inhomogeneous multiphase material soil and the interaction between soil and geothermal system. The authors conducted various studies on the heat transport and transient heat distribution in subsoil and on the thermal interaction of geothermal heat exchangers. In order to increase the prediction accuracy, extensive numerical investigations were carried out considering different thermal soil and groundwater flow properties and were validated with measurements from model tests and realized projects. Additionally to these fundamental numerical investigations on the thermal subsoil behavior, the authors' experiences with complex coupled simulations of various large urban geothermic projects including high-rise buildings are presented.

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Coupled Surface-Subsurface Modeling across a Range of Temporal and Spatial Scales
Conveners: Reed M. Maxwell, Lawrence Livermore National Laboratory; and

Mario Putti, University of Padua, Italy (putti@dmsa.unipd.it)

The interaction of groundwater dynamics, overland flow, and land-surface processes has gained recent attention in hydrologic sciences. Over the past several years, owing also to updated numerical and computational technologies, new approaches for modeling these coupled interactions have been developed. Research is addressing these issues from a range of scales and process descriptions. The goals of this session are to discuss these new techniques and to understand the feedbacks of these coupled processes across the hydrologic cycle. Contributions are invited on theoretical, numerical, and experimental studies that address all components of the water and energy cycles in an integrated fashion over a wide range of time scales (diurnal to decadal) and spatial scales (column to basin and global scales). Emphasis is placed on the coupling of the different processes of the surface-subsurface-land-surface system. Presentations are encouraged on techniques for modeling and predicting groundwater storage and fluxes on multiple scales, links to climate and global water cycle variability, groundwater remote sensing, and prospects for extending the value of existing knowledge and observational records across scales. Specific subtopics of interest include watershed dynamics, feedbacks on evapotranspiration, thermodynamics of soil moisture, infiltration and runoff, and interactions with atmospheric and precipitation processes, among others.

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Coupling finite elements and smoothed particle hydrodynamics methods for reactive transport

Authors: Yilin Fang, Timothy D Scheibe, Alexandre M Tartakovsky

Hybrid multiscale simulations are motivated by problems in which large-scale phenomena of interest (e.g., flow and contaminant transport) are strongly influenced by processes occurring at much smaller scales (e.g., diffusive mixing and reactions) that are not well represented by effective or averaged processes or properties. Executing an exhaustive simulation of processes at the smallest scales for a domain of engineering significance is currently impractical. However, the hybrid multiscale approach, in which a small-scale model with high resolution is utilized in a fraction of the overall domain and is linked to a large-scale model with coarse resolution over the remainder of the overall domain, can provide necessary efficiency of characterization and computation that will render solution of these problems practical. A hybrid approach to couple finite elements (FE) and smoothed particle hydrodynamics (SPH) methods for reactive transport is presented using a mixed interpolation for regions where finite element nodes and particles both have an influence. This approach combines the advantages of FEM and SPH. It allows high resolution simulation around the reaction front using particles and there is no need to refine the finite element mesh. Solutions using this approach will be compared to other available solutions.

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Coupling, routing, and assimilation features in a surface--subsurface catchment hydrological model

Authors: Matteo Camporese, Stefano Orlandini, Claudio Paniconi, Mario Putti, Mauro Sulis

Coupled models for the simulation of surface and subsurface flow are of increasing interest in hydrology and other Earth sciences. A variety of approaches is available for representing the dynamics on the land surface and in the stream, lake, soil, and aquifer compartments of a catchment, and for resolving the interactions between the surface and subsurface flow regimes. Process-based approaches numerically resolve the nonlinear partial differential equations for conservation of mass and momentum over the flow region of interest. In this presentation a distributed process-based model is described that includes several novel features relevant to the representation and accurate simulation of surface--subsurface processes and interactions. A path-based (rill flow) conceptualization of surface flow dynamics is used, with several options for identifying cell drainage directions and for separating channel cells from hillslope cells. Lakes and other topographic depressions are identified and specially treated as part of the pre-processing procedures applied to the digital elevation data for the catchment. Boundary condition switching is used to partition potential (atmospheric) fluxes into actual fluxes across the land surface and changes in surface storage, thus resolving the exchange fluxes, or coupling, between the surface and subsurface modules. Nested time stepping allows smaller steps to be taken for typically faster and explicitly solved surface routing, while a mesh coarsening option allows larger grid elements to be used for typically slower and more compute-intensive subsurface flow. Sequential data assimilation schemes allow the model to be updated with spatio-temporal observation data of surface and subsurface variables. These and other features are presented, and the physical and numerical behavior of the model under a variety of conditions is illustrated with five applications that cover a range of scales from 0.0027 to 356 square kilometers.

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Crystal dissolution and precipitation in porous media: variable pore geometry and upscaled model

Authors: Tycho van Noorden, Sorin Pop

In this work we propose a pore scale model for crystal dissolution and precipitation in a porous medium. Using this model we derive a macroscopic model using a formal homogenization procedure. Our investigations are motivated by the work of P. Knabner et al. ({\\it Adv. Water Res.} 1995) and C.J. van Duijn et al. ({\\it J. reine angew. Math.} 2004). We consider a porous medium that is fully saturated by a fluid in which cations (e.g. sodium ions) and anions (e.g. chlorine ions) are dissolved. In a precipitation reaction, n cations and m anions can precipitate in the form of one particle of crystalline solid (e.g. sodium chloride) attached to the surface of the grains (the porous matrix). The reverse reaction of dissolution is also possible. As a result of the precipitation and dissolution of crystals the geometry of the flow domain may change. The pore-scale model we propose consists of a system of coupled partial differential equations on a variable domain. The changes in the flow domain, which occur due to the dissolution and precipitation of crystals are modeled by a Stefan-like boundary condition. This describes the movement of the interface between the fluid and the crystal layer. For simple geometries we show that solutions of the pore scale model exist and we study their qualitative behavior using both analytic and numerical techniques. We derive an upscaled model for two different pore geometries: for a thin strip and for a perforated domain. For both geometries we perform numerical simulations and show that solutions of the upscaled model match the averaged solutions of the pore-scale model very well.

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Darcy scale modelling of biomass accumulation in the subsurface

Authors: Anozie Ebigbo, Rainer Helmig, Holger Class, Alfred B. Cunningham

A model is presented which simulates microbial processes coupled with flow and transport processes in the subsurface on the Darcy scale. The intended application of the model is to explore the feasibility of the use of engineered biofilm barriers in the context of geological carbon dioxide (CO2) storage. This could include the plugging of damaged or fractured cap rock (confining layer) in injection well vicinity in a CO2 storage reservoir, protection of well cement against corrosion by a biofilm or the creation of low-permeability zones in the geological layer above a leaky cap rock. The development of the model concept is done in two steps.The first step is the description of one-phase (water) flow and the accumulation of biomass in a porous medium. This includes the modelling of the attachment/deposition of biomass from the bulk fluid to the solid phase (grains), bacterial growth in the biofilm and in the aqueous phase, detachment (shear and sloughing) from the biofilm, the effect biofilm growth has on the porosity and permeability of the porous medium (clogging) and the transport of a growth-limiting substrate and/or electron acceptor. In a second step, the one-phase model is extended to account for a second fluid phase (CO2). In this case, the flow model describes the effect of the individual fluid phase saturations on their mobility (relative permeabilities) as well as the role of capillary pressure. On the other hand, the influence of microbial processes on two-phase flow, e.g. changes in capillary pressure and the influence of the gas-water interface on microbial processes also have to be considered. This is ongoing work. Also, other important processes such as the potentially harmful effect of supercritical CO2 on the biobarrier or the effect of high pressures (which prevail in such reservoirs) on the development of the biofilm are to be quantified and included in the model concept.

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Data Assimilation and Superposed Models for Floodplain Flows

Authors: Jerome Monnier, Joel Marin

Classical network river models are based on global-net 1D St-Venant equations, possibly with storage areas. Standard observations are available only in very small quantities in the main channel (water level measurements at very few gauging stations), while remote-sensed data such as satellite images are punctual in time but spatially distributed (eg snapshot of a flood extension). In order to take advantage of spatially distributed data and/or local data available outside the main channel (typically when flooding), we elaborate a method which superposes locally a 2D shallow-water model (the local zoom model) over the 1D global shallow-water model. The superposition (coupling 1D-2D) is done using an optimal control approach, by minimizing a misfit functional at interfaces. This approach allows to assimilate simultaneously the 2D local data into the 1D global-net model (using a variational data assimilation method, 4D-var). Thus, after convergence of the optimization process, one obtain the local zoom model coupled with the global model, and the local data assimilated into the global model (which allows the identification of inflow discharge and/or physical parameters for example). In other words, the local zoom model makes local data come back up to the global model. Numerical results show the efficiency of the method. Given data available outside the main channel only (ie not represented by the global model), one manage to calibrate the global model using the present superposition principle. Different versions of the algorithm (all based on optimal control processes) are discussed. Key Words: shallow-water 1.5D - 2D, local zoom model, variationnal data assimilation, river hydraulics, flood plain, remote sensed data. REFERENCES [1] J. Marin, J. Monnier, “Combined data assimilation and local superposed shallow-water models for surface flows”. Submitted. [2] I. Gejadze, J. Monnier, 2007, “On a 2D zoom for 1D shallow-water model: coupling and data assimilation”. Comp. Meth. Appl. Mech. Eng. (CMAME). vol. 196, issues 45-48, pp 4628-4643, 2007. [3] M. Honnorat, J. Marin, J. Monnier. DassFlow software.http://dassflow.gforge.inria.fr

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Data assimilation techniques for a coupled model of surface and subsurface flow

Authors: Matteo Camporese, Claudio Paniconi, Mario Putti, Paolo Salandin

Data assimilation in the geophysical sciences refers to a methodology to optimally merge model predictions and observations. The Kalman Filter (KF) is a statistical and sequential data assimilation technique that is optimal for linear dynamics and measurement processes with Gaussian error statistics, while for nonlinear filtering problems the Ensemble Kalman Filter (EnKF) has been demonstrated to be a suitable alternative. EnKF is a Monte Carlo approach based on the approximation of the conditional probability densities of interest by a finite number of randomly generated model trajectories. In Newtonian relaxation or nudging (NN), which can be represented as a special case of KF, model variables are driven towards observations by adding to the model equations a forcing term proportional to the difference between simulation and observation (relaxation component) and containing four-dimensional weighting functions that can incorporate prior knowledge about the characteristic scales of spatial and temporal variability of the state variable(s) being assimilated. In this study both EnKF and NN have been implemented in a relatively complex hydrological model, which couples a three-dimensional finite element Richards equation solver for variably saturated porous media and a finite difference diffusion wave approximation based on a digital elevation data for surface water dynamics. We report on the retrieval performance of the two assimilation schemes in a three-dimensional tilted v-catchment synthetic test case. The comparison between the results of the two approaches allows us to evaluate how EnKF can help to tune parameters controlling NN weighting functions and, by contrasting the way temporal information is propagated in NN, whether the lack of temporal correlation of the updates in EnKF limits this scheme's retrieval capability.

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Deposition in multiphase flow through porous media on the pore scale

Authors: Adler

Mixtures of oil and water flowing through a porous medium contain most of the times solutes which may deposit onto the solid walls. A precise analysis of this convection-diffusion process necessitates several ingredients. First, a realistic model of the porous structure is obtained by means of the method of reconstructed porous media (1). Second, the simultaneous flow of two immiscible phases can be obtained by means of lattice Boltzmann codes; the interfacial tension and the wetting properties of the solid walls can be included in the physical description of the phenomena (2). Third, the convection-diffusion of the solute can be modelled by random walks; different diffusion coefficients and a partition coefficient of the solute between the two phases can be introduced (3, 4); moreover, the deposition of the solute onto the walls can be described by a first order reaction (5). Deposition onto the walls may have two consequences that we have studied separately. In the first case, the solid phase is increased by deposition; porosity is progressively decreased until clogging occurs and stops the flow and the deposition process; during this stage all the quantities such as the absolute permeability and the relative permeabilities vary as function of time; such a situation is common in formation damage. In the second case, the solute does not clog the porous space and its only influence is to modify the local wettability of the solid walls; this may be a schematization of deposition of asphaltenes. The three ingredients necessary to study these phenomena are presented as well as the general architecture of the codes. Then, some results are presented for each case and their main features discussed. Ref: (1) P.M. Adler, C.G. Jacquin, J.A. Quiblier, Flow in simulated porous media. Int. J. Multiphase Flow, 16, 691, 1990. (2) I. Ginzbourg, P.M. Adler, Boundary flow condition analysis for the three dimensional lattice Boltzmann model. J.Physique II, 4, 191, 1994. (3) J. Salles, J.-F. Thovert, R. Delannay, L. Prévors, J.L. Auriault, P.M. Adler : Taylor dispersion in porous media. Determination of the dispersion tensor. Physics Fluids A, 5, 2348, 1993. (4) S. Békri, P.M. Adler, Dispersion in multiphase flow through porous media, Int. J. Multiphase Flow, 28, 665, 2002 (5) S. Bekri, J.-F. Thovert, P.M. Adler, Dissolution of porous media.Chem. Eng. Sci., 50, 2765, 1995.

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Design of Carbon Dioxide Storage in Oilfields and Aquifers

Authors: Ran Qi, Erica L Thompson, Tara C LaForce, Martin J Blunt

We extend our study of the design of carbon dioxide, CO2, storage in aquifers, SPE 109905, to oilfields. We demonstrate that pore-scale trapping can be an effective mechanism to rapidly render the CO2 immobile. We explore the sensitivity of the results to different trapping models through an analysis of available experimental data, one-dimensional analytical solutions and field-scale simulation. We construct analytical solutions to the transport equations, accounting for relative permeability hysteresis. We explore the impact of different trapping models and sequences of brine and CO2 injection. We design an injection strategy where CO2 and water are injected simultaneously followed by chase brine injection such that both displacement fronts are stable and the CO2 is quickly trapped. We then apply a streamline-based simulator that captures dissolution, dispersion, gravity and rate-limited reactions in three dimensions to investigate the field-scale consequences of different storage and recovery strategies. We use two reservoir models: one is a public domain model of a North Sea field (SPE10), while the other represents an oilfield for which CO2 injection is being considered. We propose a design criterion where CO2 and water are injected simultaneously such that the displacement is just stable. This is followed by the injection of brine, whose total mass is approximately 25% of the injected CO2. This approach ensures that the vast majority of the CO2 trapped while maximizing storage and, for oilfields, providing optimal oil recovery.

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Designing and implementing a framework for metadata translations using Dijkstra's shortest path algorithm

Authors: Wolf-Dieter Otte, Mike Kasper, Corinna Gries

===Summary=== The handling of data and related metadata becomes difficult when different stakeholders adopt different metadata standards. In this presentation, we will focus on the design and implementation of a framework, which allows for metadata translations, under the assumption, that the translations are entirely controllable by a set of style sheets. ===Metadata and metadata standards=== When collecting water-related data, it is particularly important to also collect the associated metadata. This metadata typically contains all the essential information describing the data itself, allowing the data to be detected, prescreened, evaluated and eventually accessed. This means, that a specific piece of data is not being made available by the owner directly, but rather described in terms of metadata. This indirection has many advantages, e.g. data does not need to be replicated, there is a high degree of flexibility in what a data provider chooses to expose, the data provider maintains control of the data, the system can grow gradually etc. In order for this approach to work, there must be a shared understanding of what metadata is, i.e. what individual pieces of information are required from a data provider. An equally important aspect is the agreement among all of the stakeholders on how to represent metadata technically. This is typically a result of setting up a standard. However, the dilemma with agreeing on a metadata standard is that often, many of these standards exist, and different groups of stakeholders may adopt different standards. This defeats the purpose of standardization and makes it hard to exchange metadata between those groups. For example, there exist at least three metadata standards for geospatial data, i.e. FGDC ("Content Standard for Digital Geospatial Metadata", issued by the Federal Geographic Data Committee), EML ("Ecological Metadata Language", a popular metadata standard issued by the "Knowledge Network for Biocomplexity") and ISO 19115. So, quite naturally, the need arises to be able to translate metadata documents between different standards. ===Developing a metadata translation framework=== The abstract model, adopted by the project, denotes any specific metadata standard (represented by its schema) as a node in a directed graph. An edge between two nodes is represented by a style sheet, which performs a one-way translation between the two standards, i.e. a "hop". In this graph, it can take several hops to get from one node to another. Some nodes might not be reachable at all. With these pieces of information, complex transformation paths can be constructed. Any achievable path can be applied to a metadata file, transforming it to the desired standard. However, in a certain transformation scenario, the ideal path is one that requires the least number of hops, i.e. the smallest number of translations. Dijkstra's shortest path algorithm is employed to find the shortest path between any two nodes, ensuring an optimal solution. The framework's behavior is solely controlled by an XML configuration file,which is provided by the module's user. The configuration file contains information about the metadata types that can be handled, as well as information on the available style sheets. This configuration file is read during runtime. Moreover, the available style sheets can be located anywhere on a network, e.g. in a style sheet repository, using any standard or non-standard communication protocol, e.g. "ftp", "http" or "xml:db" for accessing an eXist database. Unknown protocols can be used on the fly as well, as long as appropriate communication objects are made available.

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Determination of Dynamic Coefficient in Porous Media: Experimental approach

Authors: MAHSANAM MIRZAEI, GILLIANE C SILLS, DIGANTA BHUSAN DAS

The multi-phase flow behaviour in porous media is described by the relationships among capillary pressure (Pc), saturation (Sw) and relative permeability (Kr). It has been shown that conventional quasi-static equations may not be applicable in dynamic conditions when Pc strongly depends on saturation and saturation changes with time ($\partial Sw/\partial t$). The dependence of Pc on $\partial Sw/\partial t$ is known as dynamic effect. To address this issue, dynamic capillary pressure-saturation (Pc-S) relationships have been proposed which include an additional term to account for dynamic effect. The additional term has a coefficient called 'capillary damping' or 'dynamic coefficient' (τ), which establishes the speed at which flow equilibrium is reached. Despite many studies indicating the importance of dynamic effect, there are few experimental studies aimed in quantifying this, particularly in three dimensional (3D) domains. Consequently, there are significant uncertainties on the values of τ in the literature. This issue is investigated by an experimental study to establish vertical two-phase flow for drainage and imbibition of 3D homogeneous media. In this study, locally measured Pc-S curves are determined at dynamic and quasi-static flow conditions at three different heights of homogenous domains. The local Pc-S and $\partial Sw/\partial t$-t data are then used to determine experimental dynamic coefficient, τ. As expected, the results confirm that at the same saturation, the corresponding capillary pressure is higher for dynamic than for quasi-static conditions. Also, for similar transient flow conditions, the Pc-S curve for a low permeability medium lies higher than for a medium with higher permeability. The dynamic coefficient (τ), as a measure of dynamic effect, is a non-linear function of saturation and depends on porous media permeability and history of saturation (drainage or imbibition). In drainage condition, locally determined dynamic coefficient as a function of water saturation (τ-S) slightly varies from one location to the other but the functional dependence follows similar trends at different heights. Therefore, saturation weighted average of local τ-S curves is defined as an effective τ-S curve for the whole domain and follows an exponential trend. In imbibition case, however, τ-S curve does not flow a clear trend but lies higher than drainage curve.

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Determination of significant rainfall events using cluster analysis, for Mexico, using a personal computer.

Authors: Ramos Soto Juan Carlos, Montero Martinez Martin, Traversoni Dominguez Leonardo

In this work we present a new computational and statistical method, for determining rainfall patters significant for Mexico using cluster analysis, we can identify groups of precipitation in a form statistical having similarity, also shapes and spatial and temporal evolution of rainfall. Scorning the curvature of the Earth, we consider the space is as a Euclidean space. We experimented with various techniques cluster, as manhatan and euclidean distances, among others, but for our case study, let\'s take the euclidian distance. We understand these clusters, as storms, for this work we need, \"R\" program in its version 2.4.1, a database (grid) called \"MAYA\" with rainfall every 24 hours and a personal computer. The data output from \"R\" could also be helpful to make decisions on potential disaster areas. The estimation of the rain is very important for hydrology and this new statistical tool, to help us estimate, taking the conceptual model of precipitation behind this. This new tool will be very useful for rainfall-runoff models. This a basic work to be used in future work to forecast weather and climate, in addition to that will be used by the National Weather Service of Mexico Keywords: New Method, Cluster Analysis, Rainfall Patterns, \"R\"2.4.1, Euclidian Distance, Personal Computer.

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Determination of the full permeability tensor

Authors: Waltraud Kull, Olaf A. Cirpka

This work presents a new method of getting the full permeability tensor. Therefore a special construction of a three dimensional working permeameter with a corresponding numerical program is developed. And others, non hydraulic proceedings, like a magnetic and an optical method are used for comparsion so that the understanding of the three-dimensional character of permeability in the range of small and middle scale is upgraded. Usual conducted permeameter experiments according DIN 18130 are one – dimensional. The water flows only in one direction through the sample, so you get the right value of permeability of isotropic media. But every anisotropic sample, like the most natural sediments constitutes in this permeameter an apparent permeability, which is added up to dislocation from measurement direction, and the direction of the main hydraulic permeability. And we get no information about the second and the third main direction of the hydraulic permeability tensor. The new designed three-dimensional permeameter has on every side of the 0,1 m³ sized sample a filter area which can be used for inflow, outflow, closed or some special shortcuts with other sides. So a large number of different measurements combinations is possible. The selected 22 experiments with measured flux and the corresponding piezometer height on every side create and overdetermined problem. To determine the anisotropy hydraulic conductivity tensor of samples an inverse model is developed by intergrating a forward model into a numerical parameter estimation scheme. The forward model, which is working with the FEM, simulates the water flow by estimated value and built up a computational grid orientatedto the main directions. For parameter estimation we work with second-order non-linear least-square minimization scheme, the Gauss-Newton method. To obtain a more stabilized numerical procedure the Levenberg-Marquardt algorithm is applied. Finally, the sensitivities of hydraulic measurement with respect to the spatial hydraulic conductivity distribution are calculated by the adjoint state method. The model presumes homogenous characteristics of the samples. In order to investigate the reaction to heterogenous dataset, artifical randomised three dimensional filed with known qualities are feed in the inverse modelling program. The output is compared with the known qualitites of the heterogenous input. The additional magnetic technique is the Anisotropy Measurement of Suspectibility, AMS. After hydraulic investigations the samples are made smaller and the pore space is filled with ferrofluid. The magnetic particles of the fluid constitute with the measurements in 15 directions a magnetic tensor of the pore structure. The resulted tensors, the hydraulic and the magnetic one, of different natural or artifical sediment samples, as soon as some two-dimensional image analysesof the microscopic pore structure are compared.

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Developing Artificial Neural Networks to Represent Salinity Intrusion from Sea Level Rise

Authors: Sanjaya Seneviratne, Francis Chung, Jamie Anderson

Understanding potential salt water intrusion into the Sacramento-San Joaquin Delta system due to sea level rise is critical for management of California's future water supply. The Delta is the hub of California's state and federal water projects, the State Water Project (SWP) and Central Valley Project (CVP) respectively. Water released from upstream storage reservoirs flows into the Delta. Pumps in the southern Delta export the water to canals that convey the water to central and southern California. About two-thirds of California's water supply passes through the Delta system. Rising sea levels would enter the Delta though San Francisco Bay and would bring higher water levels and salinity concentrations. Water managers need methods for quantifying the increased salinity intrusion to develop strategies for protecting the Delta's future water quality and California's future water supply. The California Department of Water Resources has developed a methodology for creating Artificial Neural Networks (ANNs) to estimate salinity intrusion for sea level rise scenarios. Although simulation models can be used to estimate salinity intrusion, setting up and running the models can be time consuming. A tool to quickly assess salinity intrusion into the Delta was desired to support decision making. To meet that goal, ANNs were developed for five scenarios: (1) Future conditions without sea level rise (2) Future conditions with a 1ft increase in sea level (no change in tidal amplitude) (3) Future conditions with a 2ft increase in sea level (no change in tidal amplitude) (4) Future conditions with a 1ft increase in sea level with 4inch increase in tidal amplitude (5) Future conditions with a 2ft increase in sea level with 4inch increase in tidal amplitude. Outputs from various simulation models were used to create the data sets for training the ANNs. These ANNs correlate Delta inflows and electrical conductivity (EC), a measure of salinity, at key water quality compliance locations. The ANNs can then be incorporated into decision making tools to assess potential impacts of sea level rise on water project operations. As an initial application, the ANNs have been incorporated into CalSimII, a SWP and CVP operations model, to investigate possible mitigation measures, such as changes in reservoir releases and export pumping, to maintain Delta water quality standards. Resulting impacts to water supply can also be examined. The coupling of sea level rise ANNs with a water resources operations model provides a powerful decision support tool for managing California's future water resources.

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Development and application of a three-phase model coupling methane gas and microbial dynamics

Authors: José M. Mogollón, Ivan L\\\'Heureux, Andy Dale, Doug LaRowe, Pierre Regnier

Reactive-transport models (RTMs) of geomicrobial dynamics in subsurface environments have largely ignored the role of biogenic gas generation, transport, and dissolution. Nevertheless, a dynamic gas phase can have a direct influence on the movement of the solid and aqueous phases as well as on the rates of reaction within the system. To address this issue, a one-dimensional RTM based on mass, momentum, and volume conservation for the solid, aqueous, and gas phases has been developed. The numerical transport algorithm includes advection for all three phases as well as diffusion for dissolved components present in the aqueous phase. The geochemical reactions include interactions between the solid-aqueous and the aqueous-gas phases, as well as the possibility for microbial-mediated processes governed by thermodynamic (i.e. affinity of the reaction, departure from equilibrium) and kinetic (i.e. Michaelis-Menten) constraints. The model is validated using a natural subsurface sediment system characterized by high labile organic matter fluxes and, consequently, high rates of methanogenesis leading to methane gas ebullition. Here, the generation and transport of gaseous methane may be an effective mechanism which can sustain the microbial community carrying out the anaerobic oxidation of methane. Accordingly, the three-phase RTM is coupled to an explicit representation of the methane-using microbial community to explore the fate of methane gas in unconsolidated sediments. The model is able to elucidate the dynamics of methane bubbles and reveals important feedbacks between dissolved and gaseous methane transport and geomicrobial reaction rates.

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Development of a Sampling-based Bayesian Model for Watershed-Scale Characterization

Authors: Jinsong Chen, Susan Hubbard, Valeri Korneev, David Watson

Improving our ability to characterize, model, and monitor watershed-scale processes is increasingly important for water resources management and water quality control. In this study, we develop a characterization approach for quantitatively delineating major flow pathways within a watershed. Our focus is on the Bear Creek Valley Watershed of the Oak Ridge Field Research Center (FRC) in Tennessee. Intensive studies are being conducted at the site to explore the utility of remediation approaches to reduce and immobilize Uranium and other contaminants in the subsurface, and to quantify recharge pathways and other hydraulic drivers for groundwater flow as needed to explore their temporal variation and impact on subsurface biogeochemical conditions that are relevant to remediation strategies. Data collected at the site have indicated that a transition zone, located between the upper unconsolidated saprolite and the lower competent bedrock, is the main pathway of flow and contaminant transport, and that there may be a correlation between seismic refraction velocity and the subsurface material competency. Although surface geophysical techniques have been used for decades to characterize shallow subsurface regions, the approaches typically suffer from two main limitations. The first limitation is that the characterization is qualitative in nature and is subject to a large degree uncertainty. Typically, the surface geophysical data are inverted for geophysical attributes, which are sometimes then qualitatively associated with subsurface stratigraphy or properties. Due to the nonlinearity and non-uniqueness of the inversion processes, and to the great uncertainty associated with the petrophysical relationships that link the geophysical attributes and the hydrological properties of interest, estimating flowpaths with sufficient accuracy and certainty is challenging. The second limitation is that it is currently challenging to quantitatively integrate large amount of multi-scale data that are often available over a given watershed during the characterization process. We develop a stochastic approach in this study for watershed-scale characterization of transition zones by integrating large-scale surface seismic refraction data with several types of local-scale geophysical and hydrogeological information (such as crosswell seismic tomographic data, borehole flowmeter testing data, the depth of refusal during drilling). We integrate the multi-scale and multi-source information using a Bayesian framework to provide the estimates of the spatial distribution of the transition zone and their associated uncertainty. Within the Bayesian framework, seismic first arrivals (not the inverted seismic slowness data) are considered as input. We use a staggered finite difference method (with second order precision in time and fourth order precision in space) to forward model the full seismic waveform in 2-D with subsequent automated traveltime picking. Seismic slowness and indicator variables of transition zones are considered as unknown variables in the framework. By conditioning to the seismic traveltimes and other types of information available at different scales, we are able to estimate the probability of encountering the transition zone as a function of location and depth within the watershed.

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Development of an Iterative Site Characterization

Authors: Matthew D. Grace, Scott C. James, Thomas S. Lowry, Bill W. Arnold, Genetha A. Gray

Sparse subsurface data are insufficient to truly characterize and understand a groundwater system. Uncertainty in site characterization arises from a lack of knowledge about the site and includes uncertainty in the boundary conditions, characteristics, location, and behavior of major features within the investigation area, as well as differences in numerical implementation. In addition, site characterization often involves expert elicitation and scientific analysis to determine the most likely processes that are present. The aggregation of these processes and how they interact form the initial conceptual model. However, given the level of uncertainty associated with site characterization, improved methods are needed to guide the overall process. Previous work has applied information criteria (e.g., Akaike and Bayesian) to multi-model ranking to address conceptual model uncertainty in hydrogeologic modeling. In this work we address the iterative process of data collection and site conceptualization that is inherent in actual investigations. Gains in site understanding are tied to the combined efforts of data collection and model simulations, and ideally, these can be systematically constructed (e.g., using experimental design) to maximize the information and understanding of previous efforts. To demonstrate this procedure, a hypothetical site (namely, a complex numerical model of a hydrogeologic flow system) was developed. All observation data sets for characterization were obtained from this site. Next, a series of alternative conceptual models were developed and calibrated to data sets that were iteratively supplied from the hypothetical site. These conceptual models were ranked for each data set, and validated to evaluate a model's predictive capability before subsequent calibration with the next data set was performed. This routine contains realistic aspects of site characterization, combined with formal techniques of model selection, to improve the performance of the resulting calibrated model.

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Development of particle tracking algorithms on various types of finite elements in multi-dimensions

Authors: Heejun Suk, Gour-Tsyh Yeh

An accurate and efficient particle tracking algorithm has been developed and proposed in the Journalof Hydrologic Engineering, ASCE [in review] by Suk (2008) under complicated unsteady flow as well as steady flow conditions. In this study, in order to enhance extendibility and applicability of the previously proposed particle tracking technique, the previously developed particle tracking algorithm is complemented and modified to be performed on various types of element within finite elements in multi-dimensions. For example, the developed particle tracking algorithm incorporates quadrilateral and triangular elements in two dimensions while in three dimensions, triangular prizm element, tetrahedral element, and hexahedral element. Finally, various examples and applications are designed to illustrate that the developed particle tracking technique has wide applicability and practicality in the field of groundwater flow and transport.

Development of the Sulfidic Diffusion Active Permeable Reactive Barrier (DAPRB) Technology

Authors: Alex O. Schwarz, Bruce E. Rittmann

We have proposed (Schwarz & Rittmann, 2007) a generally applicable bioprotection mechanism by which some bacteria in a community induce pore-water metal gradients by producing ligands that bind the metal toxicant, reducing the toxicant's concentration to non-inhibitory levels for much of the community. An excellent example of this community-based bioprotection mechanism involves sulfate reducing bacteria (SRB), which produce sulfide that can coordinate toxic free metals to form solids or soluble complexes. The results of our previous analytical and numerical modeling provide evidence that microbial consortia ought to be able to use chemical gradients to detoxify a metal and criteria when the bioprotection mechanism ought to be effective. The metal-resistance criteria indicate that gradient resistance works much better in diffusion-dominated systems (e.g., sediments), compared to advection-dominated systems (e.g., aquifers). Therefore, environmental biotechnologies ought to exploit the advantage of the diffusion mechanism for metal resistance. A popular form of bioremediation today, the biotic permeable reactive barrier (PRB), is based on generation of sulfide by SRB as the groundwater moves through a permeable zone. Based on our analysis, biotic PRBs might not be the best option for toxic metal removal in aquifers, because they are advection-dominated. This insight leads us to propose a novel approach, the diffusion-active permeable reactive barrier (DAPRB). In the DAPRB, layers of low conductivity (low-K) containing reactive materials are intercalated between layers of high conductivity (high-K) that transport the groundwater across the barrier. Because diffusion dominates transport in the reactive layers, microbial communities can take advantage there of the chemical-gradient mechanism for protection from toxicants. The ideal sulfidic DAPRB design includes particulate organic matter and solid sulfate mineral inside the reactive (low-K) layer. This leads to sulfate reduction and the formation of sulfide ligands that complex with toxic metals, such as Zn2+ in the high-K layer. Using the biogeochemical model CCBATCH, which we expanded to include transport processes, we perform a quantitative biogeochemical analysis of the ideal configuration of a DAPRB for treatment of Zn-contaminated groundwater. Our analysis using the expanded CCBATCH confirms the gradient-resistance mechanism for bio-protection, with the ZnS bio-sink forming at the intersection of the Zn and sulfide plumes inside the high-K layers of the DAPRB. The detailed DAPRB analysis also shows that total alkalinity and pH distributions are representative footprints of the two key biogeochemical processes taking place, sulfidogenesis and Zn immobilization as sulfide mineral. This is so because these two reactions consume or produce acidic hydrogen and alkalinity. Additionally, because Zn immobilization is due to ZnS mineral precipitation, the ZnS mineral distribution is a good indicator for the bio-sink. Bio-sinks are located for the most part within the high-K layers, and their exact position depends on the relative magnitude of metal and sulfide fluxes. Schwarz, A. O., B. E. Rittmann (2007). Analytical-modeling analysis of how pore-water gradients of toxic metals confer community resistance. Advances in Water Resources, 30: 1562–1570.

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Dispersion and reaction in porous and fractured media

Authors: J.-F. Thovert, I. Bogdanov, V. Mourzenko, P.M.Adler

The major purpose of this work is to obtain precise numerical simulations on dispersion and reaction in these media in to order to analyze the short time and long time behaviours of solute, and to compare the results with the predictions of various theories. Three major steps are needed for the numerical solutions. First, an unstructured tetrahedral mesh of the fractures and of the porous matrix located in between is constructed; second, the Darcy equations are discretized and solved, in a finite volume formulation (1). Third, the evolution of the solute concentration has to be calculated. This last point is the most difficult one if one wants to avoid numerical diffusion. Various schemes has been tried and the most efficient one is a non linear flux limiting scheme of the Superbee type. Because of its importance, the results obtained with the various schemes will be illustrated and discussed. Then, numerical dispersion experiments were performed in a long parallelipipedic box of fractured porous medium with impermeable side walls or lateral spatially periodic boundary conditions. The number of parameters which can be studied, is very large. Basic parameters are the shape, size, orientations and density of fractures. The porous medium itself may have constant properties or not. The fracture network itself may be either mono or polydisperse (in which the probability distribution of the fracture diameters is a power law). The statistical properties of the porous medium and of the network may be stationary or not. Various effects will be illustrated such as the dispersive behaviour of fracture networks in impermeable media and such as the regularizing influence of the porous medium on this phenomenon. The output of the solute will be interpreted in terms of the various models existing in the literature (Gaussian dispersion, CTRW and fractional derivative). Finally, the solute may interact with the solid matrix. It may deposit and progressively clog the medium, or it may dissolve the solid wall and progressively increase the permeability. These two situations will be illustrated and analysed. Various effects will be analysed. References (1) I.I. Bogdanov, V.V. Mourzenko, J.-F. Thovert, P.M. Adler, \\\"Effective permeability of fractured porous media in steady-state flow\\\", Water Resour. Res. (39), 1029-1044, 2001WR000756, 2003.

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Distinguishing mixing and spreading in multiphase transport through heterogeneous media.

Authors: Jesús Carrera, Sergio A. Bea, Matthias Willmann, Orlando Silva, Luit J. Slooten, Marco Dentz, Diogo Bolster, Pablo Gamazo

Mixing describes the process by which a plume blends with resident water causing plume concentration anomalies to disappear. Spreading, on the other hand, describes the rate of expansion of a plume. Mixing causes reactions to occur. Spreading does not. Both concepts are complementary (spreading promotes mixing), but different. Yet, they are equated in the Advection-Dispersion Equation for transport. A number of alternative formulations have been developed in recent years to model conservative transport (MRMT, memory functions, CTRW, FDE). These yield residence time distributions that are in close agreement with those observed in the field. They can also be used to represent quite accurately mixing (and, thus, reactive transport) in heterogeneous media. We present an algorithm for multicomponent reactive transport in multicontinuum media. We describe a module that implements this algorithm and can be easily linked to existing flow and transport codes. We discuss its application to multiphase problems. We simulate reactive transport through a heterogeneous aquifer, using the ADE to represent local mixing. We then compare the simulated reaction rates with those obtained using the multicontinuum representation. Preliminary results show that overall reaction rates are simulated quite well.

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Downscaling of climate change projections at high spatial resolution using the method of constructed analogues

Authors: Hugo G. Hidalgo, Michael D. Dettinger, Daniel R. Cayan, Tapash Das

A Constructed Analogues (CA) method showed encouraging results for downscaling monthly precipitation (P) and average temperature (Tavg) patterns over California and Nevada. Monthly P and Tavg patterns from a coarsened version of the observations and from the GFDL model were downscaled from a 2.5 x 2.5 degree (coarse) resolution grid to a 2km x 2km (fine) resolution grid. The GFDL scenarios tested were a 20th century climate 20c3m scenario, and climate change scenarios A2 and B1. In the CA method presented here, a number (n) of analogous patterns from a "library" of previously observed climate patterns were used to construct linear estimates of the climate model target patterns. In this case, seven patterns (n=7) were used that showed to produce the highest verification correlation of the downscaled with the observations. The method is computationally undemanding, requiring only the inversion of an n by n matrix for each month. Our version of the method is also simpler than other CA implementations as no Principal Component Analysis is needed. Also, climate and trends arise from an entire large-scale weather pattern rather than being imposed GCM-grid cell by grid cell. Another advantage of the method is that it does not constrain future weather to be the same as historical. The downscaling method skillfully reproduces historical observed monthly variations of P and Tavg anomalies, as well as seasonal cycles, across the domain region. In the case of the climate change projections, the method reproduces well the magnitude of the trends in P and Tavg when compared to the raw trends in the GFDL model, but the downscaled trends show more texture associated with topography and exposure. The CA method presented here can be used to downscale output from a variety of different climate model applications. Presumably it could also be used to patch missing data, at least during the period covered by various reanalyses (1948-present). Thus, the downscaling method presented here offers many potential uses, relying where possible on the particular strengths of the large-scale models while providing flexibility for capturing unexpected changes in the large-scale climate projections and weather predictions. Future work will include running a hydrological model (e.g. the Variable Infiltration Capacity) at 2km resolution to evaluate the hydrological response of the basin to historical and climate change scenarios.

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Ecoinformatics for Water Resource Modeling

Author: Deb Agarwal, Lawrence Berkeley National Laboratory

Water resource data is now available from a broad array of government, local, and private entities. Ideally this data would be readily selectable and usable in modeling environments. However, managing and integrating these diverse datasets into a usable format and naming schema is typically a time consuming and tedious task. There are many efforts currently under way aimed at improving the usability of data in a water resource modeling environment. For this session, we solicit presentations on new and recent research into ecoinformatics techniques to enable dramatic improvements in the ease of finding, assessing, and linking hydrologic data to water resource models. In particular, we encourage submissions that address information modeling and organization of hydrologic databases and languages for exchanging water data to support water resources data and model interoperability.

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Effect of Diffusion on Dispersion and Mixing

Authors: Raman K. Jha, Steven L. Bryant, Larry W. Lake

Mixing in porous media is a complex process involving interplay of convective spreading (mechanical mixing) and diffusion. Dispersion which is used to quantify mixing is calculated from solute concentration averaged over the entire cross section of the medium. It is different from local (or “true”) mixing which is defined as homogenization of solute concentration inside a pore body. It is caused by diffusion by moving solute particles across the streamlines. This paper investigates the impact of local mixing on transmission (or forward) and echo (or backward) dispersion in porous media. We developed deterministic rules for tracing solute particles through a physically representative network model of a dense random packing of spheres. The model preserves the intrinsic spatial correlation of pore-space features. The particle flow path through the network is deterministic in the absence of diffusion, permitting us to quantify the convective spreading explicitly. We scan particle positions as a function of time and calculate dispersion coefficients from particle temporal and spatial statistics during forward as well as backward flow. We show that the longitudinal dispersion coefficient increases from a small value at the injection time to an asymptotic value at the end of a transitory period. The dimensionless dispersion coefficients obtained from network simulations match well with the experimental data for all range of Peclet numbers. We also show that only echo dispersion can differentiate between purely convective spreading and local mixing. Transmission dispersion is not affected by diffusion for moderate and large Peclet numbers. Echo dispersion is zero in absence of diffusion, but becomes non zero (and much greater than diffusion) when we include diffusion. Diffusion causes local mixing and forces solute particles to take a different path back to the inlet when flow direction is reversed, making mixing an irreversible process. The echo dispersion progressively increases with the penetration distance and finally becomes equal to the asymptotic transmission dispersion when diffusion has had enough time to cause complete local mixing. Mixing becomes independent of flow direction when complete local mixing takes place.

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Effect of heterogeneous soil and root structure on the dynamic behavior of the water budget in the vadose zone

Authors: Anna Kuhlmann, Insa Neuweiler, Sabine Attinger, Anke Hildebrandt, Sjoerd E.A.T.M. van der Zee

As the unsaturated zone is the interface between the subsurface and the atmosphere it plays an important role in climate modeling. The exchange of water is determined by infiltration, evaporation, redistribution of water and transpiration by plants. Models for water flow in the soil capture this by appropriately chosen sources and sinks and boundary conditions. In general, flow in the unsaturated zone is calculated according to the Richards equation. A challenge is that predictions of the water budget are needed for large scales but soil is highly heterogeneous on small scales, which cannot be resolved. Modeling of water fluxes with the resolution of soil heterogeneity would be computationally too demanding and would require knowledge about the soil parameter distribution, which is usually not available. It is a major goal to gain a general understanding of the relationship of heterogeneous structure of soil parameters and roots and large-scale flow processes in the soil. The poster deals with the relationship between soil and root heterogeneity and water fluxes on a lab scale, considering dynamic systems i.e. timely varying boundary conditions and sink term. Heterogeneity of soil is usually described by a parameter field with multi-Gaussian distribution. As nature is not Gaussian it is important to look at fields with more realistic structure, such as structures with connected pathways of extreme parameter values. A comparison of flow processes in multi-Gaussian fields with processes in fields with more realistic structure could improve our understanding of the applicability and the limitations of methods, which are based on a multi-Gaussian model, such as second order perturbation approximations. The relationship of soil and root structure and water budget in the soil under consideration of water uptake by roots is investigated with the numerical model MUFTE – UG, where the water exchange with the atmosphere is modeled in the following way. Infiltration due to rainfall is accounted as the top boundary condition in which the process of saturation of one cell during infiltration is modeled by a switch of Neumann to Dirichlet boundary condition. Runoff water ponds on saturated cells being distributed to non-saturated cells in the next time step. Transpiration is implemented as a sink term which is proportional to a root density distribution and with restriction in uptake due to water and oxygen deficit (Feddes-Function). Rainfall and transpiration are timely varying with different frequencies. Different settings are applied to depict the influence of soil and root heterogeneity on the water budget. Variable parameters are rainfall events with changing frequencies and different kinds of structures (Gaussian fields, fields with connected extreme values and fields with root-resembling structures) of the soil and root parameters. Different cross-correlations between root- and soil parameters are considered, in particular correlation and anti-correlation between root uptake parameters and soil parameters. Depth profiles (mean values and variance of potential, water content and sink term versus depth) and the change of total water content and total transpiration over time are compared for the scenarios mentioned above. Based on these simulations it is analyzed in the poster, which characteristic properties of soil heterogeneity influence water budgets on a large scale for a given time scale and when the approximation of multi-Gaussian parameter fields can be applied.

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Effect of slope on subsurface free-convection processes.

Authors: Ravindra Dwivedi, John L Wilson

Whether it is air or water flow in caves, or water flow in porous aquifers, geothermally-driven free convection is influenced by the geometry of the flow and heat transfer field. When the roof of a cave or tunnel, or the upper boundary of a porous aquifer, is sloping gravitational buoyancy forces interact with the slope, affecting critical Raleigh numbers, convection cell and flow field geometry, and heat and mass transfer characteristics. This interaction of slope and geothermal gradient influences the hypogenic speliogenesis of caves and the micrometerology of modern air filled caves. In porous media it influences flow and heat transfer in deep aquifers and the heat field in subduction zones. Generic simulations of these processes for both free flowing fluids and porous media are presented along with applications to speliogenesis, cave micrometerology, deep continental aquifers, and subduction.

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Effects of thermodynamically consistent threshold capillary pressures on residual nonwetting phase saturation and relative permeability

Authors: Arsalan Zolfaghari Shahrak, Mohammad Piri

Helmholtz free energy balance and the Mayer-Stowe-Princen (MS-P) method are used to find thermodynamically consistent threshold capillary pressures for two-phase displacements in capillary tubes with noncircular irregular cross-section and nonuniform arbitrary wettability. Pertinent formulations are presented for various regular and irregular cross-sectional shapes and fluid configuration changes. We adopt Kovscek wettability alteration scenario that allows any values for the advancing and receding contact angles to be assigned, permitting us to model contact angle hysteresis. We define several capillary elements with varying corner half angles and inscribed radii and assume that they are fully saturated with water and water-wet. Then we use the abovementioned techniques to compute threshold capillary pressures associated with the displacement of water by a non-wetting phase (primary drainage). We allow the wettability of the surfaces contacted by the non-wetting phase to change. The wetting phase (water) stays in the corners as wetting layer. We then compute a thermodynamically consistent threshold capillary pressure for displacement of non-wetting phase by water and define the most favorable fluid configuration. It is shown that how the threshold capillary pressure and the final fluid configuration may vary with wettability, cross-sectional shape, and the maximum capillary pressure reached during primary drainage. In all cases calculated threshold capillary pressures based on the energy balance are compared with the geometrical and snap-off capillary pressures. We then implement the algorithms in a three-dimension mixed-wet random pore-scale network model to investigate the effects of the thermodynamically consistent threshold capillary pressures on the relative permeabilities and the residual nonwetting phase saturations during water injection in systems of varying wettability, particularly water repellent systems. The model allows multiple phases to be present in each capillary element in wetting and spreading layers, as well as occupying the center of the pore space. Each displacement is modeled as a change in fluid configurations. Then a series of displacement steps in each pore or throat are combined to simulate different flow processes. Different random network models that represent the pore space in different porous systems (e.g., Berea sandstone) are used in this study. A robust displacement-based clustering algorithm is used to track the continuity of each phase-location. Using thermodynamically consistent threshold capillary pressures the two-phase relative permeabilities and residual saturations are computed. For instance, in water repellent systems nonwetting phase layer formation and collapse directly control the amount of residual saturation and the behavior of nonwetting phase relative permeability particularly in low saturations. We show how the stability of nonwetting phase layers sandwiched between water in the corner and water in the center depends on wettability and the maximum capillary pressure reached during primary drainage. It is shown that a previously used geometrical criterion for the formation of the nonwetting phase layers is required but not sufficient. The results are significantly different from those predicted using the geometrical criterion.

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Efficient calculation of large scale response to CO2 injection

Authors: Jan Martin Nordbotten, Micael A. Celia, Mark E. Dobossy

Sequestration of carbon dioxide (CO2) in deep sedimentary formations has emerged as a timely option in the global effort to mitigate anthropogenic carbon emissions. Due to the proximity to large point sources of CO2, on-shore sedimentary basins are economically and practically attractive targets for potential sequestration. However, the last 10 years have seen an increased awareness of the challenges posed by the presence of a long legacy of petroleum exploration and exploitation. This takes the form of a large areal density of active and abandoned wells, whose properties (in terms of quality of completion, location, and a lumped parameter we will refer to as "effective wellbore permeability"), may or may not be known to satisfactory certainty. Simultaneously, it is clear that sequestration of environmentally significant quantities of CO2 leads to consideration of large spatial domains, while the need for long term security motivates considering temporal domains of centuries. Thus the challenge is to tackle simultaneously: A) Large spatial and temporal domains (from 302 horizontal km2 times 3000 vertical meters times 100 years for single injection operations, to 500x100 km2 times 3000 meters times 1000 years for regional analysis); B) coupled non-linear equations whose behavior are strongly dependent on processes at the well bore scale (typically with a diameter of about a third of a meter) and C) Unknown parameters associated with wells necessitating possibly thousands of realizations in a Monte-Carlo setting. To address these challenges, we have in a series of papers developed a suite of semi-analytical solutions. Within appropriate homogeneity assumptions, this suite allows us to obtain quick and accurate analysis of the flow and pressure response to injection operations. Thus, we have a tool which can be used in analyzing the possibility and characteristics of leakage for a given injection operation. Other approaches for considering problems with strongly interacting scales are methods which fall under the label "multi-scale". One such methodology, the Variational Multi-Scale (VMS) method developed by Hughes et al., is particularly appealing due to its flexibility in application. A few authors have looked at versions of this methodology in the porous media flow context, however an implementation has yet been attempted which exploits the full flexibility of the framework. These VMS based methods are particularly well suited when considering problems with high permeability variation, however they are challenged by the need for accurate approximation to sub-space Green's functions. In this presentation, we will discuss the possibility of combining these methodologies, using a numerical VMS based approach to capture the regional flow effects on regional scales of hundreds of kilometers, and using semi-analytical approximations to form the sub-space Green's functions which are needed to accurately capture the effect of injection and leakage on the local, kilometer, scale. This will allow us to combine the flexibility of considering complex heterogeneous large scale flow fields with fast and accurate representations of local flow processes. Further, the VMS methodology inherently leads to decoupled fine scale problems for the equations we consider, a significant advantage in the design and implementation of efficient parallel algorithms.

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Efficient numerical techniques for multi-component reactive transport problems with the global implicit approach

Authors: Serge Kräutle, Joachim Hoffmann, Peter Knabner

The talk proposes some techniques for the efficient numerical simulation of multi-component reactive transport in the subsurface. Splitting techniques, solving the transport separately from the reactions (iterative or non-iterative), may be subject to considerable limitations concerning time step size or robustness or accuracy. This makes the application of the global implicit approach (GIA, one-step methods) desirable. The systems under consideration consist of PDEs and ODEs (for the mobile/immobile species concentrations), coupled through both kinetic and equilibrium reactions modeled by algebraic equations (AEs). If minerals with a possibility of total dissolution are included, the system may also contain inequalities. Due to the large size of the resulting PDE-ODE-AE(-inequalities)-system with the GIA, besides the use of parallel computers, also efficient techniques concerning the formulation of the differential(-algebraic) system can help to reduce the cpu time: (1) It is possible to concentrate the couplings and nonlinearities in a subset of the equations leading to a decoupling of some linear PDEs and thus a faster solution. The technique involves the introduction of linear combinations of the PDEs/ODEs, a linear variable transformation, and a DSA (direct substitutional approach)-like technique with respect to the new variables. The model is not simplified, but equivalently reformulated, and the transport operator remains linear during the reformulation. (2) The correct description of equilibrium mineral precipitation/dissolution requires a combination of equations and inequalities to describe both the saturated and the undersaturated situation. While state-of-the-art codes usually apply some \'trial-and-error\' strategy to determine the correct mineral assemblage, requiring several Newton iterations for one time step, it is possible to find a formulation as a complementarity problem, which can be solved by one semismooth Newton iteration. The strategies described are implemented in a software RICHY-2D running on parallel computers and have been applied to several problems, including the MoMaS benchmark problem on multicomponent reactive transport.

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Electrical Resistivity Tomography monitoring of a tracer test experiment and local hydraulic properties assessment from data

Authors: Matteo Camporese, Giorgio Cassiani, Rita Deiana, Paolo Fabbri, Paolo Salandin

In recent years geophysical methods have been used increasingly as tools for subsurface transport process characterization. For instance time-lapse electrical imaging represents a powerful tool for solute transport characterization since a full picture of the spatio-temporal evolution of the process can be obtained. This method can provide spatially and temporally highly resolved information on subsurface parameters which are closely linked to both structural and transport properties. However, a quantitative interpretation in solute tracer experiments is made difficult by the uncertainty related to the ERT data as well as to the a priori unknown hydraulic properties (e.g. porosity, hydraulic conductivity, storativity, etc.) in heterogeneous natural formations. The (arbitrary) initial state of the plume, as defined by its concentration field, also control the subsequent evolution of solute cloud. Here an approach based on the Lagrangian formulation of transport and the ensemble Kalman Filter (EnKF) data assimilation approach is suggested to analyze the cross-hole ERT data collected during a tracer test experiment performed in a fine gravel aquifer of Villorba (Treviso). The data consist of 2D cross-hole ERT images collected both longitudinally and transversly to the groundwater flow direction. The time interval between images is very small (about 20 minutes) as required by the fast dynamics of the groundwater system. Under the assumption that the solute spreads as a passive tracer, for high values of the Peclet number the spatial moments of the evolving plume are dominated by the porosity and the spatial distribution of the hydraulic conductivity. The assimilation of resistivity measurements also in terms of low – order spatial concentration moments permits the update of the system state vector that include information about the spatial distribution of hydraulic conductivity and porosity. So that the assessment of both the concentration evolution and the delineation of the local aquifer heterogeneity can be achieved at the same time by the new methodology proposed to interpret time-lapse electrical images from tracer test experiments.

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Ensemble Forecasting in Environmental Modeling

Authors: Jasper A. Vrugt, Los Alamos National Laboratory and Souheil Ezzedine, Lawrence Livermore National Laboratory

In the last few decades, much progress has been made in the use of dynamic simulation models for the analysis and understanding of environmental systems. In many fields of study, however, predictions with these models have historically focused on a single forecast, without an explicit estimate of the associated uncertainty. This broad session is open to contributions concerning methods, strategies, and applications of ensemble forecasting in environmental modeling. Particular interests lie in methods and applications of state-space filtering techniques for merging measurements with model predictions, and methods characterizing simulation uncertainty through multimodel ensembles. Examples of these include (but are not limited to) Kalman and Particle Filtering strategies, Bayesian Model Averaging and non-parametric approaches. We welcome contributions from different disciplinary fields, including water resources modeling, surface and subsurface hydrology, petroleum engineering, and climate change.

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Estimating permeability from quasi-static deformation

Authors: D. W. Vasco

Transient pressure variations within a reservoir can be treated as a propagating front and analyzed using an asymptotic formulation. From this perspective one can define a pressure \'arrival time\' and formulate solutions along trajectories, in the manner of ray theory. We combine this methodology and a technique for mapping overburden deformation into reservoir volume change as a means to estimate reservoir flow properties, such as permeability. Given the entire \'travel time\' or phase field, obtained from the deformation data, we can construct the trajectories directly, there-by linearizing the inverse problem. A numerical study indicates that, using this approach, we can infer large-scale variations in flow properties. In an application to Interferometric Synthetic Aperture (InSAR) observations associated with a CO2 injection at the Krechba field, Algeria, we image pressure propagation to the northwest. An inversion for flow properties indicates a linear trend of high permeability. The high permeability correlates with a northwest trending fault on the flank of the anticline which defines the field.

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Estimating the effects of facies heterogeneity at fine scale on the dispersion tensor

Authors: Chiara Vassena, Mauro Giudici

Heterogeneity of facies at the scale of individual lithological levels controls water flow and contaminant transport at larger scales in porous sediments. Equivalent hydrodynamic parameters of blocks of alluvial sediments from the Ticino valley (Northern Italy) whose volume is of the order of a cubic meter have been computed in a previous work (Zappa et al., Journal of Hydrology, 325, 134-153, 2006). The detailed distribution of facies (pixels with side of 2 cm) was obtained by sedimentological analysis of the boundary surfaces of these blocks; the inner 3D distribution was obtained with stochastic simulation; the conductivity (K) field was obtained by assigning different values of K to different facies; finally numerical flow modelling with standard finite differences techniques provided the equivalent K tensors for the whole blocks. Here the dispersion tensor of these sedimentary structures is estimated by application of Integrated Finite Differences modelling and of particle tracking. The following topics are analysed: (1) comparison between Eulerian (estimates from fitting breakthrough curves) and Lagrangian (estimates from second order moments of particle distributions) dispersion coefficients; (2) dependence of the results on hydrostratigraphic structures (preferential flow paths or small K levels); (3) dependence of the results on the flow dimensionality (2D vs. 3D modelling).

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Estimation of a three dimensional hydraulic conductivity field at the Rifle, CO Integrated Field Challenge site using a sequential Bayesian-Inverse Approach

Authors: Andreas Englert, Michael B. Kowalsky, Ken Williams, John Peterson, Frank Spane, Darrell Newcomer, Phil Long, Susan Hubbard

Ongoing work within a shallow (3-6m below ground surface), unconfined aquifer at the DOE Integrated Field Challenge site (IFC) in Rifle, CO focuses on stimulated bioremediation to facilitate immobilization of uranium. Previous work at the IFC showed that the injection of acetate (an electron donor) into the aquifer can stimulate bacteria to reduce mobile uranium below an acceptable limit, and that the efficacy of the stimulated bioremediation was strongly governed by the ability to deliver acetate to the location of uranium contamination. Previous hydrological inversion work showed that the acetate delivery was governed by the hydrological heterogeneity, which changed over time as precipitates and/or biomass evolved in response to the biostimulation. Although the vertical variations in hydrological properties could not be resolved with the previous datasets, the study indicated the importance of understanding how flow characteristics and biogeochemical transformations influence each other. To better understand the three-dimensional influence of hydrological heterogeneity on acetate distribution and associated biogeochemical transformations, we colleted a dense dataset of wellbore geophysical, crosshole radar, bromide tracer test, flowmeter, and slug test data within a new biostimulation flow cell at Rifle, called the \'Winchester Cell\'. This cell, which is 4m by 3m in size and includes 10 injection and 15 monitoring wells (three upgradient and twelve downgradient), was used subsequently to conduct a one month stimulated bioremediation experiment. Here, we present a methodology that we developed to efficiently utilize all hydrogeophysical datasets to estimate hydraulic conductivity and associated uncertainty within a 3D grid that encompasses the Winchester cell. The approach involves the sequential application of Bayesian and hydrological inverse methods. In a first step, a Bayesian method is used to integrate wellbore flowmeter and slug test data with crosshole radar datasets to provide estimates of hydraulic conductivity and associated uncertainties at each voxel in the Winchester cell. In a second step, these posterior estimates are used as prior information for inverse modeling using the iTOUGH2 code, a pilot-point method and the bromide tracer test data. Through comparison of the Bayesian estimation results with those obtained using the sequential Bayesian-Inverse approach, we assess the value of the sequential method for incorporating all relevant hydrological data and the advantage of delineating the vertical variations in hydraulic conductivity for understanding field transport.

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Estimation of gas permeability field in landfills using inversion modeling

Authors: Yoojin Jung, Paul Imhoff, Stefan Finsterle, Ramin Yazdani, Don Augenstein

Operating bioreactor landfills requires optimizing the moisture content for microorganisms to rapidly transform and degrade organic waste while simultaneously capturing the landfill gas (LFG) generated. Bioreactor operations typically involve the controlled addition of water or leachate and efficient capture of LFG. In order to control the simultaneous movement of water and gas, there is a pressing need for better models to describe fluid flow in bioreactor landfills. Such models depend on characterization of the permeability field. However, the highly heterogeneous structure of waste results in preferential flow, making it difficult to estimate the spatial variation of the permeability field using only point measurements and deterministic approaches. A methodology to estimate the gas permeability field for refuse in landfills is evaluated using inversion modeling with appropriate field data. The pilot point method is selected for this purpose and is implemented in iTOUGH2. To improve the accuracy of estimated parameters, the joint use of different data sets is considered: gas pressure changes in response to pumping rate changes, and gas tracer test data. In addition, the use of a dual-porosity model is evaluated to account for matrix/channel flow patterns that are hypothesized to occur in many landfills. This study will be the first application of this inversion procedure to landfill data. The methodology is expected to aid management of LFG collection in bioreactor landfills.

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Evaluating model predictions and characterization methods applied to the deep vadose zone at San Gorgonio Pass, California: Lessons learned after 5 years of artificial recharge

Authors: Alan Flint, Kevin Ellett, Allen Christensen, Peter Martin

The hydrogeology of the unsaturated zone plays a critical role in determining the suitability of a site for artificial recharge. Optimally, a suitable site has highly permeable soils, capacity for horizontal flow at the aquifer boundary, lack of impeding layers, and a thick unsaturated zone. The suitability of a site is often determined by field and laboratory measurements of soil properties, field experiments, and numerical modeling. In 2000 borehole instrumentation was installed in an existing, but unused, artificial recharge site in the San Gorgonio Pass area in southern California, USA. This allowed for long term for field measurements and observations to characterize the site and develop a conceptual model of the unsaturated zone. A numerical model was developed using TOUGH2 on the basis of the conceptual model and was calibrated using data from a 50-day artificial recharge experiment conducted in 1991. Results indicated that a restrictive layer exists 250 feet below land surface that would cause lateral diversion of the artificially recharged water, thus greatly reducing recharge to the water table 650 feet below land surface. The results of these investigations were published in 2004. In the summer of 2003 artificial recharge was initiated and continued on and off until the spring of 2007. Data collection from the instrumented boreholes also continued and wetting front arrival times, changes in the elevation of the perched water at 250 feet, and a rise in the water table at 650 feet have provided the data necessary to reevaluate the conceptual model. The computer model was updated and model parameters refit to the new data collected during active artificial recharge using inversion techniques and the inversion code iTOUGH2. The perching layer appears to be about 3 times more permeable than original interpretations suggested, and the lateral hydraulic conductivity above the perching layer appears to be about an order of magnitude less permeable, which is potentially related to a fault thought to exist down dip of the recharge ponds. The implications of these updated interpretations may indicate that more recharge may occur under the ponds that originally thought although significant movement down dip may still cause recharge to occur further down dip into the saturated zone.

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Evaluation of climate change impacts on water resources of Ebre River Basin with GIS-BALAN

Authors: Javier SAmper, Diego ALVARES

Abstract Here we present an evaluation of the impacts of climate change on water resources in several catchments of the Ebre River Basin in Spain. Hydrological models have been calibrated using data collected from 1970 to 2000. Simulations were performed for IPCC scenarios A1B, A2, B1 and Commit using projection outputs from global climate model CGCM3 and for the following periods: 2010-2040, 2040-2070 and 2070-2100. A computer code, GENBALAN, was developed for statistical downscaling of CGCM3 monthly results and dis-aggregation of monthly to daily series. A semi-distributed hydrological code, GIS-BALAN, has been used to perform water balance in selected catchments. Model results of climate change impact show a marked space-time variability and indicate an average decrease in total runoff of 16.2%, 23.8% and 18.2% for simulation periods 2010-2040, 2040-2070 and 2070-2100, respectively. Impacts will be more severe in Southern basins which already show the most intense water deficits.

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Evaluation of High-Resolution Piezocone Methods for Site Characterization and Groundwater Modeling

Authors: Amvrossios C. Bagtzoglou, Jessica Furrer Chau, Mark Kram, Gary Robbins

A site at Port Hueneme Naval Base in California, USA, has been characterized using the US Department of Defense's Site Characterization and Analysis Penetrometer System (SCAPS), obtaining soil type, porosity, hydraulic head and hydraulic conductivity data at high spatial resolution. A 10 ft by 25 ft area was sampled at 5 foot intervals, and readings were collected at high (1-inch) vertical resolution at each push site. The resulting borehole data was used to generate two alternate conceptual models of the site stratigraphy, using conventional stratigraphic principles and Markov chain transitional probabilities based on soil type readings. This conceptual model was the basis for a three-dimensional GMS groundwater model of the site, and various methods of interpolation have been employed to create alternate realizations of the hydraulic conductivity field. We contrast the results of standard 3-D kriging of SCAPS hydraulic conductivity estimates, co-kriging with soil type, and Markov chain transitional probabilities in generating hydraulic conductivity fields for the flow model. To evaluate the accuracy of the realizations, a pumping test was performed, with a forced-gradient tracer test planned for the final analysis of stratigraphy realizations. Results of the modeling of the pumping test are presented.

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Evaluation of Model Coupling Frameworks for Use by the Community Surface Dynamics Modeling System (CSDMS)

Authors: Scott D. Peckham

The Community Surface Dynamics Modeling System (CSDMS) is a recently NSF-funded project that represents an effort to bring together a diverse community of surface dynamics modelers and model users; this includes the hydrologic modeling community. Key goals of the CSDMS project are to (1) promote open-source code sharing and re-use, (2) to develop a review process for code contributions, (3) promote recognition of contributors, (4) develop a "library" of low-level software tools and higher-level models that can be linked as easily as possible into new applications and (5) provide resources to simplify the efforts of surface dynamics modelers. The architectural framework of CSDMS is being designed to allow code contributions to be in any of several different programming languages (language independence), to support a migration towards parallel computation and to support multiple operating systems (platform independence). In addition, the architecture should permit structured, unstructured and adaptive grids. A variety of different "coupling frameworks" are currently in use or under development in support of similar projects in other communities. One of these, ESMF (Earth System Modeling Framework), is primarily centered on Fortran90, structured grids and Unix-based platforms. ESMF has significant buy-in from the climate modeling community in the U.S.; a closely-related framework called OASIS4 has been adopted by many climate modelers in Europe. OpenMI has emerged from the hydrologic community in Europe and is being evaluated for the NSF-funded CUAHSI project. OpenMI is primarily centered on the Windows platform and the programming language C# (C-sharp) and is not oriented toward parallel computing. A third, DOE-funded framework called CCA (Common Component Architecture) achieves language interoperability by using a multi-language compiler called Babel. It fully supports parallel computation and virtually any operating system. Babel currently supports six programming languages, including C, C++, F77, F90, Java and Python with more languages planned for future releases. CCA has also been shown to be interoperable with ESMF and MCT (Model Coupling Toolkit) and would appear to be interoperable with OpenMI if C# language support were to be added to Babel. The recent addition of a new development tool called Bocca greatly simplifies the use of CCA. For all of these reasons CCA is very attractive as a base framework for the CSDMS project. This talk will present a comparison of several different coupling frameworks and will provide a demonstration of how component-based software can be developed within the CCA framework.

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Evaluation of Segmentation Techniques for Quantitative Analysis of X-Ray CT Images of Geological Materials

Authors: Pavel Iassonov, Markus Tuller

Three-dimensional imaging techniques such as Computed Tomography (CT) provide a non-destructive means for obtaining a wealth of information regarding porous structures of geological or artificial materials. However, results of two- and three-dimensional analysis of pore structures are heavily dependent on the segmentation step used to separate pore space from the surrounding solid matrix. Therefore, the choice of segmentation technique is crucial to our ability to accurately and reliably determine pore network features such and porosity, topology, pore size distribution and flow properties. In this study, we tested several segmentation methods for binarization of CT images of geological materials. A variety of well-established and recently developed techniques ranging from simple image histogram shape and global thresholding to advanced locally adaptive techniques based on geostatistical analysis were implemented and tested. Several methods for correction of common CT image artifacts such as beam hardening were also developed. Geometrical and topological pore network properties were determined based on mathematical morphology operations, and then compared not only among different segmentation methods, but also to experimentally and analytically obtained values.

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Expediting ensemble simulation using very fast statistical surrogates for high dimensional physics-based models

Authors: Sergey Frolov, Antonio Baptista, Todd Leen, Rudolph van der Merwe, Zengdong Lu

Ensemble simulations and iterative optimization with physics-based numerical models are increasingly used to estimate the state of the environment, to estimate poorly known model parameters and forcings, to characterize the uncertainty of models, and to optimize resource management using model-based control. Although traditional physics-based models provide a high-fidelity view of the environment, they often require significant computational resources, making them poorly suited for the new applications in ensemble and iterative simulations requiring hundreds of model simulations. To expedite ensemble-based simulations in computational oceanography, we recently developed nonlinear model surrogates that are trained to approximate a high-fidelity nonlinear model at a fraction of the original model's computational cost. A nonlinear model surrogate is a statistical regressor, trained to predict the future state of the model based on the previous time history of model states and forcings. We used several machine learning techniques to implement such nonlinear regressors, including a multi-layer neural network and a mixture of linear regression models. To enable training of these regression models on a physics-based model with millions of computational elements, we first reduced the state-space of the model using Empirical Orthogonal Functions. We used the developed model surrogates to implement a fast data assimilation (state estimation) system for a circulation model of the Columbia River estuary and plume. The original numerical model solved shallow water equations for the baroclinic flow in the estuary and plume on an unstructured numerical grid with ~10^7 computational elements. The data assimilation system was implemented using an ensemble-based Kalman filter, which estimated water levels, salinity, temperature, and velocity fields in the estuary and plume using sparse observations of water levels, salinities, and temperatures. Our validation experiments showed that data assimilation was successful in reducing model errors and predicting the uncertainty of the modeling system. Our data assimilation system is currently used for operational forecasts of the Columbia River estuary and plume and for optimization of the Columbia River observing system. In this presentation, we will first present a short tutorial on the model surrogate technology, followed by an application of the model surrogates to a data assimilation task in the Columbia River estuary and plume.

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Experimental and Numerical Investigations of CO2 Injection into Saline Formation

Authors: Amir Riaz, Yildiray Cinar, Hamdi Tchelepi

We present experiments and pore network simulations at the laboratory scale to investigate the influence of gravitational, viscous and capillary effects on the CO$_2$ injection process. Two-dimensional experiments are performed in a vertical glass-bead pack, in the parameter range of practical flows, i.e. with Bond numbers of about 10^{-3}, and capillary numbers of the order 10^{-4}. Experiments are carried out primarily to demonstrate the type of flow regimes that occur under favorable as well as unfavorable conditions of density and viscosity. Experiments demonstrate the existence of pore scale instability in the presence of unfavorable gradients of viscosity and density, and as such, appear to be incapable of being modeled by conventional means. A comparison with estimates from percolation theory shows good agreement with experimental observations. Numerical results from pore network simulations show that the important parameter regimes are not captured by this method. We propose a new approach to formulate more acurate flow models at larger scales.

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Experimental and Numerical Studies to Evaluate the Dependence of Accuracy of Subsurface Model Calibration on Quality and Quantity of Observations

Authors: Christophe Frippiat, Toshihiro Sakaki, Tissa H. Illangasekare

The collection of field data for aquifer characterization still often relies on very general guidelines, and few systematic approaches are available to assist the modeler in gathering useful data either through traditional methods (e.g. pump and tracer tests) or emerging hydrogeophysical techniques for the calibration subsurface flow and transport models. The goal of this work is to investigate how model prediction accuracy improves with the types and quantity of data used for calibration. It is our contention that theories and methods that will be developed in these types of studies cannot be validated in the field, as existing field characterization methods are not able to provide accurate information on the spatial distribution of the aquifer properties. In this research, we use such data from a synthetic aquifer constructed in a three-dimensional test tank with carefully controlled boundary conditions and synthetic data generated numerically. The synthetic aquifer was constructed using five well-characterized sands. The heterogeneous packing consists of two regions with different structures. The first region is a stationary spatially correlated random field. A structured heterogeneity was introduced by embedding a second region, a large homogeneous block of fine sand. Three pumping tests were conducted. The pressure distribution within the tank and the discharge rates at the well and at the tank outlet were monitored. During a series of tracer tests, fluorescein was injected at five different locations, under natural gradient conditions. A 19-channel Fluorimeter was used for automated measurement of tracer concentrations at selected point locations. Four models of the spatial distribution of the five sands were generated: the first model exactly corresponds to the distribution used for packing, while the other models are random geostatistical realizations created from three sets of borehole core data. In the field, such data could be obtained e.g. from borehole geophysical logs. The amount of boreholes included in each set varies, yielding geologic realizations with different levels of quality. T-PROGS (Transition Probability Geostatistical software) was used to generate the realizations, which were incorporated into numerical models for flow and transport built using MODFLOW and MT3DMS. The estimation of the hydraulic conductivity of the five sands was achieved by coupling the codes with the inversion code UCODE 2005. The hydraulic conductivities of the five sands were estimated for the four geologic realizations, using various quantities of observation wells. In a first calibration exercise, experimental data on steady-state drawdowns and concentration was used as observations. Transient drawdowns could not be used for this calibration exercise. The transient changes in drawdowns were observed to be very quick, and could not be recorded with a reasonable accuracy by the scanning pressure measurement device that was used in the experiments. Hence, a second calibration exercise was performed using numerically generated synthetic data sets for the same aquifer conditions as in the tank packing. Parameter estimations were performed using synthetic steady-state and transient drawdowns, and synthetic breakthrough curves. As expected, the accuracy of the calibrated model improved with the quality of the data representing the geologic realization. However, model accuracy was not found to improve steadily as a function of the quantity of observations. Rather, it usually reached a prediction error limit, reflecting both uncertainty of the geologic realization and measurement errors. This study suggests that in field investigations, the amount of data to be gathered from pumping and tracer tests should therefore be determined in conjunction with the quality and the quantity of data that may be able to be gathered through geophysically based investigations and other methods used to construct the geological model.

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Extended Metadata Registries (XMDR) for Water Resource Modeling

Authors: John L. McCarthy, Bruce Bargmeyer, TBA

This oral presentation will describe the Extended Metadata Registry (XMDR) Project, Collaboration, and Prototype and their relevance to water resource modeling. Good water resource modeling depends on reliable data and information about that data -- i.e., metadata. As data collections become more extensive and complex, water metadata itself needs to be organized and managed systematically, with careful regard to concepts and terminologies. The Extended Metadata Registries (XMDR) Project at Lawrence Berkeley National Laboratory, is a collaboration with the Berkeley Water Center (BWC) of UC Berkeley. BWC is collecting a variety of hydrological and related data from many different sites throughout California. These data, along with related metadata and concept systems, are an excellent exemplar of many semantic management issues that the XMDR project is addressing. With support from the Environmental Protection Agency, National Science Foundation, Department of Defense, and others in the U.S., Europe and Asia, we have developed a multi-national, multi-agency collaboration to help understand semantic requirements of metadata, to develop prototype software that can help inform those requirements, and to codify such requirements in a new edition of the ISO 11179 Metadata Registry Standard. In order to test and demonstrate the utility of extending metadata registries to include and manage more structured semantic information from concept systems, the XMDR project has developed a modular architecture and an open source software implementation of that architecture that can be used and extended by other individuals and organizations without cost or licensing. The XMDR project also has obtained diverse examples of \"traditional\" metadata registries as well as concept systems ranging from relatively small terminologies to very large ontologies in order to test prototype capabilities. Example prototype contents currently include over one million XML instances of different types of 11179 \"Identified Items.\" The most recent version of the implementation of our open source software, installation instructions, and example content are downloadable from our public web site Interested users can also try out our web-based prototype loaded with selected content at xmdr.org. We are currently exploring the possibility of adding a number of inter-related sets of data, metadata, and concept systems about water, such as data proposed for the Water Information System for Europe (WISE) and data in the EPA STORET system, which contains water concepts, quality, biological, and physical data that is both created and used by state environmental agencies, the Environmental Protection Agency (EPA), other federal agencies, universities, private citizens, and many others. By providing tools to help harmonize, integrate, search, and analyze different types of data from many different sources, the XMDR project is helping build the necessary cyberinfrastructure that can help address a number of important societal issues related to water, including - disaster reduction - integrated water resource management - ocean and marine resource monitoring and management - weather and air quality monitoring, forecasting and advisories - biodiversity conservation - sustainable land use and management - public understanding of environmental factors affecting human health - energy conservation

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Facies Connectivity and Conductivity Modeling

Authors: Mohsen Masihi, S. Sadeghnejad, S. Bazrafkan, Peter R. King

Oil reservoirs have a complicated geometries with heterogeneities appears on all scales from microns to kilometers. Proper modeling of the spatial distribution of these heterogeneities is crucial affecting all aspects of flow and consequently the reservoir performance. We have recently proposed a fast methodology (compared to the CPU demanding conventional approach) based on percolation theory (SPE 100333, CMWR XVI 189) to model connectivity of low to intermediate net-to-gross reservoirs. However, simple geometries such as rectangles in 2D or cubs in 3D may not appropriately represent the sandbody objects. In this paper we first use the same approach of modeling the reservoir connectivity but using ellipsoid bodies instead. We investigate numerically how this improvement can influence the threshold and the connectivity behavior although this increases the computation efforts as an appropriate optimization procedure required for ellipsoids intersection checking and also to calculate the volume occupied by all ellipsoids. Secondly, we extend the applicability of percolation approach to model the interwell conductivity. To simplify the computations, we consider single phase flow on the system. Governing flow equations are then solved for a given system size using method of control volume. This is then repeated for a large number of realizations using different system sizes to calculate the effective permeability. From the numerical results the universal conductivity exponents was found to be 1.2±0.03 in 2D and 2.1±0.13 in 3D. We have then applied the known scaling laws from percolation theory to rescale the effective permeability (conductivity) results. We have observed that the average conductivity results are collapsed onto a unique master curve with which we can estimate the average conductivity between two wells in different reservoir sizes with different net to gross ratios very rapidly. Moreover, the master curve for the associated uncertainty in the conductivity results has been determined. As a result these may be used for uncertainty assessment and decision-making of real field problems.

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Factors Controlling Groundwater Contamination from Underground Nuclear Tests

Authors: A. F. B. Tompson, R. Maxwell, S. Carle, M. Zavarin, D. Shumaker, G. A. Pawloski

Increasing concern about radioactive contamination of groundwater from underground nuclear tests has reinforced the need for a basic understanding of how the residual radionuclide inventories of such tests enter and migrate through groundwater. As a basis for studying these processes, the physically and thermally disturbed geologic environment produced by such tests and its relation to the post-test distribution of radionuclides is reviewed from a conceptual and simulation-based perspective. These concepts are being used to support the development of the "Hydrologic Source Term (HST)" in which groundwater flow and reactive transport models are used to evaluate the nature, rate, and extent of radionuclide contamination in near field groundwater surrounding specific underground nuclear tests at the Nevada Test Site (NTS). Such models have been used to evaluate HST behavior in fractured volcanic rock (Pahute Mesa), fractured carbonate rock (Yucca Flat), and porous alluvium (Frenchman Flat) environments at the NTS, under both saturated and partially saturated conditions. They can be particularly dependent on the residual (post-test) pressure, saturation, and temperature distributions in near field areas, and can pose strikingly complex simulation challenges. Ultimately, these models are being used to provide a rational basis from which defensible migration assessments over larger spatial and temporal scales can proceed. LLNL-ABS-400504. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This work was performed in support of the U.S. Department of Energy National Nuclear Security Administration Las Vegas Office Underground Test Area Project.

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Fate and Transport of Radionuclides in the Environment: Unique Simulation Challenges

Author: Andrew F.B. Tompson, Lawrence Livermore National Laboratory

This session will focus on unique simulation challenges posed by efforts to understand and manage the fate and transport of radionuclides in the environment, as specifically related to (1) high-level nuclear waste repository design and (2) the evaluation of long-term impacts of nuclear testing on water resource systems. As dissimilar as they may seem, both topics involve (a) consideration of large, multiscale hydrologic regimes (e.g., as influenced by geologic heterogeneity), (b) problem-specific hydrothermal or other multiphase flow issues, (c) model and parametric uncertainty concerns, especially in locally altered (engineered or otherwise) environments, (d) reactive transport of multiple radionuclide species in such systems, and/or (e) strict regulatory or design requirements, all of which serve to increase the complexity, data requirements, and validation needs of the simulation process. In turn, increased computational complexity will drive needs for fundamental improvements in algorithm design, sensitivity, and optimization strategies, and the kinds and ways in which field data are acquired, interpreted, and otherwise used to support these efforts. Thus we seek contributions that address one or more of these complexities in the context of the focal session topics.

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Field Scale Dispersion of Reactive Substances in Groundwater: Spreading versus Mixing Effects

Authors: Maria E. Malmström, Sten Berglund, Deguo Kong, Georgia Destouni

Many environmentally important systems involve complex water-rock interactions within natural subsurface systems that exhibit large physical and (bio)geochemical heterogeneity. The timing and duration of water pollution and the concentration levels of contaminants downstream of the pollution source are then governed by the complex interplay between (bio)geochemical reactions and physical transport along spatially variable water flow paths. Longitudinal solute spreading along the flow path occurs due to subsurface heterogeneity on various scales. Molecular diffusion and pore-scale dispersion additionally cause mixing of aqueous solutions. The objective of this study is to quantify and compare separate and coupled effects of mixing and spreading on the resulting dispersion of reactive contaminants downstream the pollutant source in a physically heterogeneous aquifer. In this study, the flexible and widely used PHREEQC code (Parkhurst and Appelo, 1999) is used to quantify (bio)geochemical reactions and 1D advective transport. In a first model approach, transport is conceptualised as taking place in a single streamtube, which is transversely fully mixed. Effects of physical heterogeneity, causing flow variability, and molecular diffusion as well as pore-scale dispersion is considered through a dispersion term, impying a large-scale longitudinal mixing of components. In another approach, the LaSAR-PHREEQC model (Malmström et al., 2004) is used. In this, the transport domain is resolved into a set of streamtubes, characterized by individual residence times for water from the source plane to the observation plane. The flow velocity along each individual streamtube and among the different streamtubes is considered to vary randomly, representing spreading of solutes, without mixing of the aqueous solutions. As case studies, we consider the reactive transport of acid mine draniange (AMD) and petroleum hydrocarbons (BTEX) in groundwater. In the case of AMD, we consider the reactive transport of potentially harmful metals, focusing on Zn2+, along with pH buffering in an anoxic groundwater. Along with the long-term physical spreading of pollutants, we account for sorption and dissolution/precipitation reactions at local equilibrium (see Malmström et al. 2004, 2008). In the BTEX case, we focus on Benzene and consider the dissolution of pollutants in originally oxic groundwater and the downstream, reactive transport. Benzene is degraded by microorganisms using dissolved molecular oxygen, nitrate, or sulphate as the terminal electron acceptor, following the approach of Prommer et al. (1999). The BTEX degradation follows Michaeli-Menton kinetics and is coupled to aneraobic and aerobic microorganism growth and metabolism. Parts of microorganisms may undergo passive transport, thereby allowing for a spatially and temporally dynamic population in the model. In the AMD case, Zn2+ is shown to be considerably retarded by the geochemical reactions. Whereas reactions coupled with mixing decrease contaminant dispersion, due to formation of reaction fronts, reactions coupled with spreading tend to increase the contaminant dispersion, through reaction front fingering. In the BTEX case, the development of the benzene plume is strongly dependent on the microbial reactions. However, the differences between the effects of mixing and spreading are not as pronounced as in the AMD case. The results of this study thus show that using a single dispersion term, neglecting the different effects of spreading and mixing, may introduce important model uncertainty in some reactive transport cases. References Malmström M.E., Destouni G., and Martinet P. (2004), Environ. Sci. Tech. 38, 2673-2679 Malmström M.E., Berglund S., Jarsjö J. (2008) Appl. Geochem. In print Parkhurst D.L. and Appelo C.A.J. (1999), USGS Water-Resources Inv. Report 99-4259, USGS, Denver, Colorado, USA Prommer H., Barry D.A. and Davis G.B. (1999) Env. Mod. Software 14: 213-223

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Field-Scale Control Volume/Test Cell to Advance Parameter Estimation and Flow and Transport Modeling with Geophysics, Boise Hydrogeophysical Research Site

Authors: Warren Barrash, Tom Clemo, William Clement, Bwalya Malama, John Bradford

The Boise Hydrogeophysical Research Site (BHRS) is a wellfield designed to support hydrologic and geophysical research with the near-term goal of developing methods for mapping three-dimensional (3D) heterogeneous distributions of permeability in coarse-grained sedimentary aquifers by combining geophysical data (indirect but abundant, inexpensive, and minimally- or non-invasive) with hydrologic data (direct or indirect but sparse, expensive, and invasive). The approach for meeting this goal is to thoroughly characterize a field-scale control volume/test cell in a natural heterogeneous fluvial aquifer where the 3D distributions of geologic, hydrologic, and geophysical parameters – and relationships between them – are being determined, and then to develop methods to jointly invert geophysical and hydrologic data for the permeability distribution. The BHRS is located on a gravel bar adjacent to the Boise River; the aquifer at the BHRS is shallow and unconfined. 18 wells were cored through 18-21 m of unconsolidated, coarse (cobble and sand) fluvial deposits and completed into the underlying red clay. The wells and the wellfield were designed to permit a wide range of hydrologic and geophysical testing and to capture short-range geostatistical information. In the central area of the BHRS (~20 m diameter), 13 wells are arranged in two concentric rings around a central well. In addition to providing local well density for single-well logging and profiling, this design provides numerous well-pair transects for crosshole tomography, and provides overlapping volumes for multiwell/multizone hydraulic and tracer tests. Data from any given crosshole or multiwell test can be related to tests through the same space with other methods, and to higher resolution, higher density data (e.g., core analysis; borehole geophysical logs; permeability, seismic, and GPR profiles) at the same wells used in a given crosshole or multiwell test. Similarly, surface geophysical lines run between wells can be related to well data and crosshole transects through the same space. Results to date from numerous methods of investigation indicate that the coarse sediments may be subdivided into five hydrostratigraphic units in the central portion of the BHRS, and that porosity and permeability vary both abruptly and gradationally within and between these units. Porosity data derived from neutron logs are highly correlated with radar and seismic data; possible petrophysical or functional relationships are being investigated. Recent experiments have tested new technologies for determining the 3D distribution of permeability (hydraulic tomography), for combining tracer testing with time-lapse crosshole radar attenuation tomography, time-lapse ERT, and combined hydrologic tests with self-potential and ERT measurements to return the distribution of thickness-averaged permeability by jointly inverting the hydrologic and geophysical data. Going forward, opportunities exist to use the BHRS as a research asset for the community where legacy data may support investigations elsewhere and where hydrologic, geophysical, or combined hydrogeophysical experiments may be conducted to test theories and models and to develop methods.

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FINITE VOLUME MODEL FOR BOD-DO INTERACTION IN STREAMS

Authors: ZULFEQUAR AHMAD

Streams are used as sinks for the disposal of domestic, agricultural and industrial wastes. In recent years, more concern has been raised on quantitative understanding of fate of the pollutants for the effective control of pollution in streams. An established measure of water pollution is the biochemical oxygen demand (BOD). The dissolved oxygen (DO) in river is of particular interest from a regulatory standpoint because water quality standards are expressed in the terms of DO. A minimum value of DO in streams is required to ensure the ecological health of the receiving water. Accurate prediction of BOD and DO is crucial to the effective management of water quality of riverine systems. Introduced into the field of computational fluid dynamics in the beginning of the seventies, the finite volume method has in recent years evolved as a powerful tool for solution of open channel flow problems. BOD-DO interaction modeling in a stream is described by a set of coupled one-dimensional transient partial differential equations, which consider the effects of advection, dispersion and sources and sinks. A finite volume (FV) model for the solution of the coupled equations using well-tested QUICK scheme is developed. For the computation of gradients of diffusion term and cell values of the advective term, the quadratic upstream interpolation for convective kinetics (QUICK) scheme is used. The scheme is third order accurate on a uniform mesh and converges to a grid-independent solution with substantially fewer grid points and requires the least computational time for a given level of accuracy. The proposed FV model is validated with the available analytical solutions for various initial and boundary conditions. The proposed FV model leads to solutions that compare well with analytical solutions. The model is for both transient and steady state conditions and inherently conservative, transportive and also do not fail at the discontinuities in the concentration field.

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Finite Volume Model For Coupled Simulation Of 1D-river Flow, 2D-overland Flow and 3D-variably Saturated Flow

Authors: Mukesh Kumar, Chris Duffy

Surface-water, vadose zone and groundwater are linked components of a hydrologic continuum. The coupled processes interact at a variety of spatio-temporal scales influenced in part by the heterogeneity in topography, climate, land-use and hydrogeology. In order to comprehensively and accurately capture the interaction between different components of a hydrologic continuum, full physical coupling, "natural" numerical coupling and parsimonious but accurate data coupling is needed. Here we present a physically based, spatially distributed hydrologic model that incorporates all the three coupling strategies. Physical coupling between 1D river flow, 2D surface overland flow and 3D variably saturated subsurface flow has been performed by implementing continuity assumption in head and fluxes at respective river-surface-subsurface interfaces. All the physically coupled components are numerically coupled through semi-discrete form of ordinary differential equations, which define each hydrologic process, using a cell-centered finite volume based approach. Multidimensional reconstruction of state variables on each control volume has been employed to achieve second-order spatial accuracy and to prevent nonphysical oscillations. The fully implicit BDF method with Newton-Krylov iteration is used to solve for all the state variables simultaneously at each adaptive time steps thus providing robustness, stability and accuracy. The accurate data coupling is aided by the use of constrained unstructured meshes, which have distinct advantages over structured grids, as they are able to conform to arbitrary geometries and their concentration can be adaptively changed in high gradient regions or in regions of particular interest in a flow field. The spatial adaptivity of the decomposed domain and temporal adaptivity of the numerical solver facilitates capture of varied spatio-temporal scales that are inherent in hydrologic process interactions. The surface flow numerical model is based on diffusive wave approximation of hyperbolic Saint Venant equations thus resulting in parabolic equations which are easier and faster to solve numerically. Subsurface flow simulation is based on solution of the complete three-dimensional nonlinear Richards equation throughout the whole flow domain. The model is able to simulate subsurface flow in heterogeneous and anisotropic geologic settings and has the capability to simulate pumping and delayed yield effects. Model performance is evaluated by reproducing the results of controlled numerical experiments for each individual processes and their interactions with that obtained from models such as VS2D, ModHMS, ParFlow and InHM. The numerical results obtained from the model are in good agreement with the ones presented in existing literature. The community hydrologic model and the associated domain decomposition toolsets developed in this effort are open source and can be used by anyone for research purposes

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Finite volume scheme for anisotropic diffusion operators : how to delete oscillations?

Authors: Christophe Le Potier

In the framework of nuclear waste disposal simulation, we are interested in a transport model in porous media which can be described by a convection-diffusion equation. Recently, a cell-centered finite volume scheme has been proposed to discretize the diffusion operator (Le Potier C., Finite volume monotone scheme for highly diffusion on unstructured triangular meshes, C. R. Acad. Sci., Ser. I 341 (2005) 787-792). We have shown the robustness and the accuracy of the algorithm in comparison with analytical solutions. This scheme satisfies the minimum or the maximum principle but not the two principles simultaneously. Let us recall, that to our knowledge, there does not exist linear scheme satisfying these principles, without geometrical constraints on the mesh and conditions on the diffusion operator. This a crucial problem, particulary in the case where the transport model is coupled with nonlinear chemical models. We propose a new algorithm which satisfies such properties for any anisotropic tensor on unstructured triangular meshes. The main idea is to calculate the gradient using a nonlinear scheme. For parabolic or elliptic problems, the resulting global matrix is an M-Matrix without geometrical constraints on the mesh and restrictive conditions on the anisotropy ratio. The efficiency of the algorithm is demonstrated by comparing it with numerical schemes which do not satisfy discrete minimum and maximum principles.

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Flow and radionuclide transport calculation arround nuclear waste disposal

Authors: Alain GENTY, Christophe LE POTIER

Modeling of radionuclide migration in geological formations is of first importance in the context of high-level nuclear waste repository safety calculations. Radionuclide transport calculations in geological repository need to describe, in three dimensions, objects of the meter scale like waste packages, embedded in geologic layer formations of kilometer extension like host rock and aquifers. A complete and basic refined spatial description of the repository design would end up with at least meshes of hundreds of millions to tens of billions elements. The resolution of this kind of problem is today not reachable with classical computers due to resources limitations. Although parallelized computation appears as potential tool to handle such kind of multi-scale calculations, to our knowledge, no attempt have been yet performed. Among others, a possible solution to repository safety calculations on very large cells meshes consist in using a domain decomposition approach linked to massive parallelized computer calculation. In this approach, the repository domain is divided in small elementary domains and flow and transport calculations are performed independently on different processor for each elementary domain. In order to develop such approach, an important question must be adressed: what is the spatial discretisation (or the number of cell) needed to perform calculations of a good (or given) accuracy level? In this paper, we present calculations of radionuclide migration on different level of refined description of a small part of the repository including meter scale objects and hundred-meter scale object constituted by host-rock geological layer. The small repository part considered can be seen as an elementary domain part of futur domain decomposition appproach. The real 3-D geometry of the repository components is used. The considered small part of the disposal is extracted taking into account the numerous symmetries of the repository design. Repository components represented are thus gallery backfill, excavated damaged zone surrounding repository cell and gallery, plug sealing the repository cell and clay host-rock. The used mesh is therefore limited to less than fiew millions elements on which calculations are feasible. Heterogeneities of the repository and interactions between scales are thus taken into account during the transport calculation. It is to note that only transport in host rock is considered and that we do not model surrounding aquifers. Flow and transport calculations in highly heterogeneous and anisotropic systems can present numerical problems. In this study we performed a series of calculations on different level of mesh refinement with a revisited Finite Volume (MPFA) spatial scheme. We compared the results to the ones given by calculation using the more classical Mixed Hybrid Finite Element (MHFE) spatial scheme.

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Flow within a Steep Forested Hillslope in Northern California

Authors: Rohit Salve, Alessandro Uccelli, William E. Dietrich, Inez Fung

While it is recognized that bedrock groundwater is a contributor to the hydrology of hill-slopes, very little is known about how water from the overlying soil moves into, and is distributed through the rock profile. We have instrumented a steep forested catchment to investigate the hydrology along the soil-bedrock continuum. The site, which is located within the Elder Creek Watershed in the Angelo Coast Range Reserve (CA) (http://angelo.berkeley.edu/visiting.htm), is dominated by winter storms from the ocean and summer dry spells. Using a combination of established techniques (e.g., Time Domain Reflectometry) and a proof-of-concept measurement system, we are monitoring moisture in both soil and the underlying bedrock (up to a depth of 2.0 m) at high spatial (centimeters) and temporal (minutes-hours) resolution in multiple locations. The hydrology of the deeper rock profile is being evaluated with a series of boreholes that intercept an underlying water table. We are developing a modeling approach that will incorporate the complex interactions between the vadose zone and the groundwater in order to better understand the moisture dynamics observed in the field. This effort is part of a larger project (The Keck Hydro-Watch Project) the long term goal of which is to gain a predictive understanding of the lifecycle of water.

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Flowing Fluid Temperature Logging in Boreholes: A Novel Approach for Estimating The Transport Properties of Fractured Porous Media

Authors: Sumit Mukhopadhyay, Yvonne W. Tsang

Borehole temperature logs provide useful information about the subsurface thermal structure. Consequently, they have been used for determining subsurface thermal conductivity and lithology and for monitoring coupled heat and fluid flow through fractured rock. Since not all the fractures intersected by a borehole contribute to the flow process, borehole logging performed under non flowing conditions is not always useful for fracture detection and property estimation. Tsang et al. [1990] introduced a flowing fluid electrical conductivity log to identify fractures that contribute to flow. More recently, Tsang et al. [2007] introduced a flowing fluid temperature logging (FFTL) for characterizing unsaturated fractured reservoirs. In FFTL, air (containing water vapor) is pumped from a borehole located in unsaturated fractured rock. As air enters the borehole from the surrounding fractured rock, it undergoes a change in pressure and gives rise to a temperature signal that can be measured. The depths in the borehole of the signals mark the locations of the hydraulically conducting fractures. The magnitude and time change of the temperature signal contain unique information for determining permeability and other transport properties. Estimation of permeabilities from FFTL is a relatively new approach. In this paper, we present the theoretical basis needed for analyzing and interpreting FFTL data. We first present a simplified model of FFTL assuming single-phase flow of air, and constant pressure and temperature inside the formation. It is also assumed that heat transfer occurs via convection only (i.e., conductive heat transfer is ignored). Based on this simple model of FFTL, we develop a semi-analytical solution for spatial and temporal variations in pressure and temperature inside the borehole. Using this semi-analytical solution, we propose a method for estimating the effective fracture continuum permeability. Our method reproduced the fracture continuum permeability from a synthetic FFTL with known permeability. We also applied the proposed method to estimation of permeability from an actual FFTL conducted in the unsaturated fractured welded tuff of the Drift Scale Test, conducted at the underground Exploratory Studies Facility of Yucca Mountain, Nevada. The effective fracture continuum permeability estimated from our method is comparable to previous independent estimates of fracture permeability. We also conducted numerical model studies. Using a numerical model of multiphase flow of air and water vapor, and heat transport by conduction and convection (based on the TOUGH2 simulator) we estimate the most sensitive parameters controlling FFTL. We use the optimization code iTOUGH2 to quantify the uncertainties associated with these parameters. Our study shows that permeability, porosity, and thermal conductivity can be estimated from FFTL. We found that two other parameters have strong influence on FFTL. These are the initial pressure and temperature in the borehole (at equilibrium with those of the rock formation). Finally, our numerical study shows that the uncertainties associated with the estimated transport parameters can be reduced with further refinement of the model (e.g. incorporating atmospheric variations in pressure and temperature within the model.) Our study demonstrates that FFTL has significant potential for determining the location of flowing fractures and the associated parameters. In this context, we are encouraged by the emergence of high-precision distributed temperature sensing systems (DTS). DTS allows collection of temperature data continuously over an entire borehole with a precision of 0.01oC or less. DTS-based FFTL will also eliminate the logistical difficulties of conventional FFTL, where the logging tool must be moved from location to location as one logs an entire borehole. In short, FFTL, backed by DTS, has great potential to be a viable method for estimating transport properties.

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Fracture Roughness Effects on Flow Through a Fracture

Authors: Dustin Crandall, Duane H. Smith

Fractures have been widely recognized as providing preferential pathways in low permeability geological media, and thus the proper characterization of these conduits is crucial for reservoir modeling of groundwater flow, CO2 sequestration, and the storage of nuclear wastes. Modeling of fractures as parallel plates within the reservoir is a widespread practice due to the large number of fractures and the computational costs of doing otherwise. However, fracture roughness has been recognized as having a dramatic effect on the fluid transport through fractures. This study evaluates the effect of fracture roughness on the effective aperture, permeability, and small-scale transport properties, to determine the level of spatial resolution required to accurately describe flow through a fracture. The computations used a computer-tomography (CT)-scanned fracture in Berea sandstone. High-resolution, finite-volume simulations, with one million or more grid cells, were used to evaluate flow through the fracture. The roughness of the fracture walls was varied by performing a series of smoothing operations on the original, 240 micron voxel resolution, CT-scanned fracture. Six 'roughness' levels were evaluated to determine the effects of fracture roughness. The levels ranged from the original scanned model to a nearly parallel plate model. Parallel processing was used to obtain the results in a reasonable amount of time, with up to 12 processors used for each case. The single- phase flow of water was first evaluated. These initial studies show a dramatic decrease in the permeability and effective aperture with the inclusion of zero-aperture regions, with the fracture walls in contact. The small- scale vector field reveals a high degree of channeling within these rougher models, and a Lagrangian particle tracking scheme was used to show that the tortuosity of the fluid flow path is greatly increased when this level of fracture roughness is included. The variation in flow properties from a nearly parallel plate geometry to a sinuous fracture model with few zero-aperture locations was not nearly as dramatic, indicating that the regions where the fracture wall touch have the greatest effect on fluid transport properties within fractures. Preliminary two-phase, immiscible flow, finite-volume simulations have been evaluated with these fracture geometries, as well. The saturation of the invading fluid was observed to decrease with the increased fracture roughness, due to the fluid preferentially moving within high-flow channels and being occluded by zero-aperture locations. Experimental studies through a realistic physical model of the sandstone fracture have been conducted as well, and these show good agreement with the simulation results. These two-phase simulations also employ parallel processing, but remain computational expensive due to their unsteady nature and high level of grid refinement.

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Fuzzy Systems Modeling for Uncertainty Prediction in Water Resources

Authors: Boris Faybishenko

The uncertainty in hydrogeological predictions often results from the imprecision, ambiguity, or vagueness of the input data used for characterizing flow and transport processes in heterogeneous subsurface and for constructing detailed models. One of the fundamental limitations of currently used deterministic and stochastic hydrogeological methods to describe subsurface processes is related to their inability to use perception-based information. The application of this information could serve as the basis for a complementary approach: fuzzy-systems modeling for assessing the uncertainty in hydrogeological simulations. Fuzzy-systems modeling does not replace conventional deterministic and stochastic simulation methods, but rather makes more sophisticated use of the information obtained using these methods. Moreover, both deterministic and stochastic analyses of subsurface processes can generally be considered complementary to fuzzy-systems modeling. The fuzzy-logic approach to modeling of a hydrogeological system is based on the assumption of imprecise boundaries between different parts of the media. Parameters such as hydraulic head, water flux, hydraulic conductivity, hydraulic gradient, porosity, and saturation can be represented as fuzzy numbers. The probability distributions of spatial (and/or temporal) variations of these parameters can be used to generate fuzzy membership functions for these parameters. The relationships between fuzzy variables—for instance, hydraulic pressure and water content versus hydraulic pressure—can be described by fuzzy functions. Fuzzy membership functions can also be used to characterize the degree of heterogeneity in a subsurface system. Using the basic concepts of fuzzy systems calculations and fuzzy granulation, a fuzzy form of the water-balance equation for evaluating the distribution of the various components of watershed hydrological balance is developed. Using this equation, examples of the evaluation of evapotranspiration, net infiltration, and groundwater recharge are shown. Using the fuzzy forms of Darcy\'s law and Richards' equation, examples of water travel-time calculations as a fuzzy variable and a fuzzy water balance for the unsaturated-saturated soil profile are presented. Fuzzy membership functions of different hydrological variables are used to represent the degree of uncertainty in water-balance simulations. This work was partially supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

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Gas-water-rock interactions at Mt. Amiata geothermal field as natural analogues for enhanced geothermal systems (EGS) operated with CO2

Authors: Fabrizio Gherardi, Giovanni Gianelli, Tianfu Xu, Karsten Pruess

A novel concept for enhanced geothermal systems (EGS) was proposed recently that would use CO2 instead of water as heat transmission fluid. Modeling studies have indicated that CO2 has very favorable properties for heat extraction and transmission to the land surface. EGS with CO2 would consist of three zones, (1) a central zone in which all aqueous phase that may have been present initially has been removed by dissolution into the flowing CO2 stream, (2) a peripheral zone in which the pore fluid is a two-phase mixture of aqueous and CO2-rich phases, and (3) an outer zone in single-phase aqueous conditions with dissolved CO2. The present paper considers the CO2-rich geothermal system at Mt. Amiata in Tuscany (Central Italy) as a potential analogue for the peripheral and outer zones of an EGS operated with CO2. Field observations of mineral alteration and fluid chemistry are used to constrain reactive chemical transport simulations, and to obtain insights into rock-fluid interactions in EGS with CO2. The high-enthalpy Mt.Amiata geothermal field consists of two main geothermal areas, Bagnore and Piancastagnaio. Two main reservoirs have been identified in the area with very different temperatures. The shallow reservoir, located at depths of 400 to 1000 m below sea level (b.s.l.), is hosted in carbonate and anhydritic formations of the Tuscan Nappe unit, and is characterized by temperatures ranging from 160 to 220 °C. The deeper reservoir at about 3000 m b.s.l. is hosted in fractured and permeable formations of the local metamorphic units, mostly chlorite phyllites and graphite phyllites of Paleozoic age. Here, the temperatures range from 250 to 360 °C. Wells produce a two-phase mixture, while liquid-dominated conditions prevail at depth. With PCO2 values up to 36 bar at reservoir conditions, the Mt.Amiata geothermal system can be considered a typical example of a high-gas geothermal field. Data from well cuttings and cores were available to define mineral abundances and hydrothermal alteration in the geothermal system, while the initial mineralogical composition of the rocks of the deep reservoir could be determined from outcrops and samples from unaltered locations. The initial chemical composition of the reservoir fluids was estimated through chemical modeling. These data were used to explore physico-chemical mechanisms likely controlling the geochemical evolution of the reservoir, with particular reference to the relationship between the mineralogical transformations and the propagation of CO2-dominated gas fronts. Numerical simulations with TOUGHREACT reveal that CO2-driven reactivity can explain many observed mineralogical features. In particular, the presence of the assemblage quartz + plagioclase + carbonate + mixed layer phyllosilicates + muscovite + K-feldspar has been successfully predicted. However, there are some complicated spatial patterns of dissolution/precipitation that call for mechanisms other than the simple advancement of a CO2-rich gas front. Mixing of waters of different composition could likely be invoked to explain such features.

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Geochemical Reactive Transport Modeling of Boiling/Evaporative Dryout in Porous/Fractured Rock

Authors: Guoxiang Zhang, Nicolas Spycher, Eric Sonnenthal, Carl Steefel

The proposed high-level nuclear waste repository at Yucca Mountain, Nevada, consists of waste-emplacement tunnels in fractured, unsaturated volcanic tuffs several hundred meters above the regional water table. The current design of the repository calls for a heat load (from radioactive decay) resulting in temperatures above the boiling point of water for hundreds of years around the tunnels, under pressures remaining essentially near atmospheric values. Therefore, the simulation of thermal-hydro-chemical processes in and around tunnels requires the capability of handling boiling and evaporation of pore water (moisture) up to conditions of extreme dryness, as well as the salt precipitation accompanying this process. To do so, new process models were developed and implemented in TOUGHREACT, an existing general-purpose geochemical reactive transport simulator: (1) a Pitzer ion-interaction model handling geochemical processes of concentrated brines, (2) an iterative algorithm solving for the equilibrium salt-brine-gas system, at which the water activity in a brine equals the air relative humidity above the brine, (3) the coupling of vapor-pressure lowering induced by salinity to multiphase flow effects, and (4) a normalized gas transport solver to simulate the transport of trace-amount gases, such as HCl and HF, which can be generated under conditions of extreme evaporative concentration. The developed process models are verified and validated against experimental data and the results of an existing well-tested geochemical reaction path code, EQ3/6. The extended simulator is used to model water-rock-gas interactions caused by boiling and evaporation within and around nuclear waste-emplacement tunnels at the proposed Yucca Mountain repository. The coupled thermal, hydrological, and chemical processes under consideration consist of water and air/vapor flow, evaporation, boiling, condensation, solute and gas transport, formation of highly concentrated brines, precipitation of deliquescent salts, generation of acid gases, and vapor-pressure lowering caused by the high salinity of the concentrated brine. The main findings from this modeling effort are as follows: (1) the near-field and in-drift brine chemical evolution is dominated by the precipitation of NaCl, CaSO4, and CaCO3; and (2) the generation of HCl gas at high evaporative concentration yields acid gas amounts that are too small to create highly acidic condensate, with predicted pH values staying >5 in condensation areas; (3) the salinity of waters in areas of highest liquid flux above modeled tunnels (taken to represent potential in-drift seepage) remains relatively low (<0.1 m NaCl). These types of simulations are useful for the long-term safety assessment of the underground repository.

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Global Implicit and Operator Splitting Methods for Reactive Transport Revisited

Authors: C.I. Steefel

While the global implicit approach for reactive transport problems has been discounted by some as an option for multi-dimensional, multicomponent reactive transport (Yeh and Tripathi, 1989), it was shown as early as 1994 that the approach was viable for hydrogeochemical transport problems (Steefel and Lasaga, 1994). In this contribution the topic is revisited in the context of the MoMaS (Mathematical Modeling and Numerical Simulation for Nuclear Waste Management Problems) benchmarks, which include a set of 1D and 2D reactive flow problems of varying complexity. All the problems include strong aqueous and surface complexation under equilibrium conditions, while some additionally include kinetic or equilibrium-controlled mineral precipitation and dissolution. Performance of the global implicit (coupling of reactions and transport using a direct substitution approach) and operator splitting (solution of the reaction and transport terms sequentially) are compared in terms of both accuracy and computational efficiency. The code CrunchFlow (Steefel, 2008), which includes the global implicit or operator splitting approaches as a runtime option, is used for all simulations. The results in 1D and 2D demonstrate that the aqueous and surface complexation problems can be handled accurately and efficiently with the operator splitting approach and a time step corresponding to a Courant number of 1. CPU times for the operator splitting approach are typically about a factor of 2.2 times faster than the global implicit approach using the same time step. To avoid operator splitting error, however, it is necessary to limit the time step to a Courant number of 1 in the case of the operator splitting approach, while the global implicit is capable of solving the problem with minimal loss of accuracy at higher Courant numbers (2-10), thus improving its computational efficiency substantially. Operator splitting error also increases for problems in which mineral dissolution and precipitation are included, so the accuracy of the global implicit approach is actually higher in these cases even using the same time step. Steefel, C.I., A.C. Lasaga, (1994) A coupled model for transport of multiple chemical species and kinetic precipitation/dissolution reactions with application to reactive flow in single phase hydrothermal systems, American Journal of Science 294, 529-592. Yeh, G.T., V.S. Tripathi, (1989) A critical evaluation of recent developments in hydrogeochemical transport models of reactive multichemical components, Water Resources Research 25, 93-108.

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Grain-scale Modeling of Capillarity-controlled Displacements in Fractionally Wetted Porous Media

Authors: Siyavash Motealleh, David DiCarlo , Steven L. Bryant

Oil reservoirs and soil are often heterogeneously wetted (mixed wettability or fractional wettability). In mixed-wet reservoirs the mechanism of wettability alteration means that a single grain can have patches that are water-wet and patches that are oil-wet. In fractional-wet porous media each grain is either oil-wet or water-wet. The water-wet or oil-wet grains are distributed randomly within the porous medium. Understanding the configuration of menisci within fractional-wet porous media is essential for developing the geometric and mechanistic criteria for displacement of one phase by another in fractionally wetted porous media. These criteria afford useful insight into the general problem of capillarity-controlled movement of menisci in porous media. We adopt an invasion percolation approach, in which displacements proceed as a series of jumps through pore throats and from pore bodies. Trapping of either fluid occurs when no path of pores connects that fluid to an exit from the medium. The pore throats and bodies are determined uniquely by the known spatial locations of the grains comprising the porous medium. We analytically solve for stable interface locations in individual throats as a function of capillary pressure, contact angles and the wettability of each of the grains defining the throat. This leads to a generalization of the Melrose criterion previously validated for pore-level imbibition events in strongly wetted media. The results yield a set of purely geometric, mechanistic criteria for menisci movement. We illustrate them in 2D media (packings of disks) and describe the extension to 3D. We compare our simulation results for macroscopic properties such as capillary pressure curve and relative permeability curves with relevant experimental results reported in the literature. A distinctive shift in the drainage/imbibition curves occurs as the fraction of oil-wet grains increases beyond a threshold value. The threshold is associated with the emergence of a percolating cluster of oil-wet grains across the domain. Phase trapping also exhibits a strong dependence on the fraction of oil-wet grains.

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Hierarchical Simulation Of Biofilm Growth Dynamics In 3-D Porous Media: Constant Flow Rate Versus Constant Head

Authors: G. E. Kapellos, T. S. Alexiou, S. Pavlou, A.C. Payatakes

Many bacteria are able to attach, grow and eventually form biofilms at the interface between an aqueous phase and another fluid, solid or even porous material, if favorable local environmental conditions persist. The term biofilm is used to describe a microbial consortium dispersed in a hydrogel of extracellular polymeric substances (EPS), and attached on a surface. The ability of certain biofilm-forming microbial species to degrade detrimental chemical species is driving the interest of scientists and engineers in studying techniques based on microbial biofilms, such as natural attenuation of contaminants dissolved in the groundwater, and treatment of waste water in porous medium based bioreactors. The analysis of biofilm growth in porous media is not trivial since the process under consideration is inherently multiscale, meaning that the different length scales interact strongly to produce the observed behaviour. We have recently developed a hierarchical simulator (HiBioSim-PM) that predicts: i) the structural and biological heterogeneity at the biofilm scale, and ii) the pattern of evolution and the rate of growth of heterogeneous biofilms within the pore space of porous media (core scale) (Kapellos et al., 2007a). In this work, we present an improved version of this simulator. The simulator includes: (1) a novel physically-constrained cellular-automaton model for biofilm proliferation, (2) a recently developed effective-medium approximation for the calculation of the local hydraulic permeability and diffusion coefficients within the biofilm as functions of fundamental geometric and physicochemical properties of the system at the cell- and EPS-scale (Kapellos et al., 2007b), (3) a Lagrangian-type simulation for detachment, re-entrainment, and potential re-attachment of biofilm fragments, (4) a novel, simple model for the calculation of the critical fluid shear stress for biofilm detachment as function of the local EPS concentration, (5) the numerical solution of the Navier-Stokes-Brinkman and continuity equations for the determination of the velocity and pressure fields in the pore space, and (6) the numerical solution of the convection-dispersion-reaction equation for the determination of the spatiotemporal distribution of dissolved carbon source (organic contaminant) and electron acceptor (oxygen) in the pore space. The simulator is used to investigate the differences in the pore scale clogging mechanism under two different core scale flow modes: constant flow rate and constant head. The simulations are performed within the pore space of 3-D virtual cores. The results are discussed in the context of experimental observations. REFERENCES Kapellos, G.E., Alexiou T.S., Payatakes A.C., “Hierarchical Simulator of Biofilm Growth and Dynamics in Granular Porous Materials”, Adv. Water Resources, 30(6-7), 1648-1667 (2007). Kapellos, G.E., Alexiou T.S., Payatakes A.C., “A Multiscale Theoretical Model for Diffusive Mass Transfer in Cellular Biological Media”, Mathematical Biosciences, 210 (1), 177-237 (2007).

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High-Resolution Numerical Approaches for Subsurface Flow and Transport

Author: John B. Bell, Lawrence Berkeley National Laboratory

High-fidelity simulations have the potential to provide valuable insights into subsurface flow and transport phenomena such as CO2 sequestration, the long-term fate of surface contaminants, and the storage of nuclear wastes. However, realizing this potential poses a number of computational challenges. Groundwater simulations must encapsulate a broad range of scales. Multiple chemical reaction fronts must be captured while simultaneously representing large-scale bulk groundwater flow. Simulations must provide an accurate treatment of multiphase, multicomponent flow with a large number of reactive species to accurately represent the geochemistry. Improving the resolution of subsurface flow and transport simulations involves a number of elements. The starting point for high-fidelity simulations is the basic discretization scheme used to accurately represent the underlying physical processes. Improvements in resolution can be obtained by developing adaptive mesh-refinement approaches that can dynamically focus computational effort in regions requiring increased accuracy. Finally, numerical approaches for high-fidelity simulation need to effectively harness the power of high-performance parallel computers.

For this session, we are seeking contributions that address novel numerical approaches aimed at improving the fidelity of subsurface flow and transport simulations, including but not restricted to such topics as high-resolution discretization methods, adaptive mesh refinement, and the solvers and software systems needed for high-performance parallel computing.

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High-Throughput Genetic Characterization of Environmental Bacteria

Authors: Adam Deutschbauer, Morgan Price, Paramvir Dehal, Jennifer Kuehl, Romy Chakraborty , Julia Oh, Ronald W. Davis, Terry C. Hazen, Adam P. Arkin

The ability to sequence genomes far outpaces our ability to systematically determine gene function. Subsequently, systems-level analyses of most environmental bacteria are limited by the presence of numerous uncharacterized genes and an over reliance on annotations from well studied bacteria such as E. coli. To meet these challenges, we are applying three genetic techniques to assess gene function in environmental bacteria: (1) custom multiplex microarrays for gene expression, (2) custom tiling microarrays for transcript identification, and (3) the parallel phenotypic analysis of thousands of sequence-defined mutants using a molecular barcoding strategy. Importantly, the described techniques are universal to virtually any sequenced and cultured microbial species, rapidly applicable without the need for extensive infrastructure, and comprehensive over the entire genome. The application of these techniques will enable the rapid dissection of stress response/metabolic pathways, improved annotation of genomes, insight into bacterial evolution at unprecedented resolution, and the linkage of field observations to those in the laboratory. Here we describe our experimental results in the context of the Environmental Stress Pathway Project (ESPP), a multi-investigator DOE-funded project with the long term goal of heavy metal bioremediation at contaminated sites. Using the metal reducer Shewanella oneidensis MR1 and the sulfate-reducer Desulfovibrio desulfuricans G20 as models, we will describe how laboratory insights derived from our high-throughput genetic data can be used to improve field models of bioremediation and hence aid in the rational engineering of complex biogeochemical processes.

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Higher-order adaptive algorithms for subsurface flow

Authors: Ann S. Almgren, John B. Bell, George Pau, Michael J. Lijewski

High-fidelity simulations of subsurface flow play an important role in assessing the long term fate of groundwater contaminants around waste disposal sites, evaluating strategies for carbon sequestration and a variety of other applications. Here, we describe a computational framework for high-fidelity simulation of multiphase-multicomponent flow in porous media. Our approach is based on a sequential formulation that treats pressure implicitly combined with a semi-implicit treatment of convection, diffusion and reactions. The convective component of the discretization uses a second-order variation of Godonov's method that provides a robust and accurate treatment of nonlinear waves. This basic discretization methodology is integrated into a parallel adaptive mesh refinement framework. The adaptive refinement strategy is based on a hierarchical approach using structured grids. The parallelization of the methodology is based on a coarse-grained distributed memory model in which grid patches are distributed to processors. We briefly describe the elements of the discretization approach and discuss the issues associated with incorporating the basic discretization methodology into the adaptive framework. Finally, we demonstrate the overall methodology and discuss parallel performance on some representative model problems.

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Homogenization of two-phase flow processes in porous media with different structures

Authors: Insa Neuweiler

Modeling of two-phase flow phenomena on large scales in natural porous media is important for many technical applications such as soil remediation schemes or storage of substances in deeper formations as well as for flow and transport processes in the unsaturated zone. When modeling two-phase flow it is one of the main challenges to capture the influence of heterogeneous substructure, which is not resolved by a model and which is mostly not known in detail. As two-phase flow is a highly nonlinear process, models to predict spatially averaged variables, which rely on linear behavior and the assumption of small parameter contrasts are restricted in their applicability. Upscaling of two-phase flow is also challenging because the assumption that the form of the model remains unchanged by the averaging process (as it is for example well established for single phase flow) does not necessarily hold and averaged models can become extremely complex and involve many parameters. One important aim of upscaling of two-phase flow and related transport processes is thus to identify flow regimes (quantified for example by dimensionless numbers and measures for heterogeneous structure of the soil), where certain types of flow models can be applied. Homogenization theory is one method to identify such flow regimes. The method is based on an expansion in terms of the relation of the typical length scale of heterogeneity (such as a macroscopic REV) and the length scale of the medium. As an example, the scale expansion applied in homogenization theory provides a tool to identify criteria for the applicability of local equilibrium assumptions. The effective parameters of upscaled models can be calculated explicitly only for very simple structures of heterogeneity. In general one would like to estimate parameters based on characteristic properties of a heterogeneous field. For two-phase flow and transport processes the information about connected or isolated parameter ranges is a very sensitive measure for heterogeneity. First because parameter contrasts can be very high, connected extreme values can dominate the flow patterns. Second, the trapping of non-wetting fluid or the temporary trapping of wetting fluid depends on whether areas with given parameters are connected to the mobile fluid phases or isolated. Upscaled models and estimation of effective parameters will be discussed for the Richards equation and counter-current two-phase flow. The upscaled models are derived with homogenization theory. In particular, the conditions for memory effects will be discussed. Effective parameters for the models are estimated based on connectivity of given parameter ranges. Connected parameter ranges are estimated from the two-point cluster density of two-cut indicator fields (Torquato et al. 88). This measure allows for estimation of trapping and thus for the estimation of macroscopic residual saturations. Differential effective medium theory is used to estimate effective parameters for the models. The method is based on the description of the heterogeneous medium as a composite with one background material. By assigning the background to the connected material, connectivity can be taken into account. Upscaled models for different structures of heterogeneous fields will be compared, in particular multi-Gaussian fields will be compared to non-Gaussian fields. References: S. Torquato, J.D. Beasley and Y.C. Chiew, Two-point cluster function for continuum percolation, J. Chem. Phys., 88(10), 6540-6547, 1988.

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Hydraulic Retroaction of Porosity change in Reactive Transport

Authors: Leterrier Nikos, Trotignon Laurent, Cochepin Benoît

Reactive transport simulations in porous media usually use a pre-defined Darcy velocity, whether it is imposed or obtained from a previous simulation of hydraulics. Yet, neglecting the retroactive effect of porosity change on the Darcy equation may lead to important errors and non-physical behaviour. An important decrease of the porosity will locally slow down the Darcy velocity, and therefore the convective fluxes. This may have important consequences in self-healing systems (e.g. clay/concrete interface in waste disposals) or at very reactive interfaces like permeable reactive barriers. When this phenomenon is not taken into account, the decrease of the porosity will be compensated by an artificial increase of the concentration of convected species. This retroactive effect on Darcy velocity was implemented in the Alliances numerical platform (co-developed by CEA, ANDRA, EdF). Alliances is designed for solving general problems in porous media, involving coupled phenomena such as hydraulics, transport, chemistry or mechanical constraints. The reactive transport problems are solved by coupling a transport and a chemical module through various techniques such as Picard or non-linear conjugate gradient algorithms. For our problem, calculation of new Darcy velocities at each time step was implemented before the Picard iterations. This numerical development is validated by comparing experiment results and simulations. First, we present the numerical simulations conducted with Alliances of a one-dimensional reactive transport experiment involving a column in which dissolution of calcite and precipitation of smithsonite and gypsum occur, leading to a strong clogging of the porosity. Taking into account hydraulic retroaction in the simulation leads to consistent results with experimental data. When neglecting it, it creates an artificial overshoot in tracer concentration and non-physical results. A two-dimensional version of this clogging experiment is now in preparation in order to explore a system in which strong directional changes of the fluid velocity field are triggered. The dimensioning of this experiment is now finalized and has been used as a numerical benchmark between three reactive transport-codes (Alliances, Crunch and Hytec). These three codes use different numerical approaches and algorithms but the predicted evolutions are in good qualitative agreement in spite of the high non linearity of the studied system.

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Hydrogeophysics: Parameter Estimation and Evaluation of Flow and Transport Models

Author: Niklas Linde, ETH Zurich

Geophysical data that are sensitive to hydrological properties or dependent variables can provide independent information in hydrological modeling and inversion studies. Successful applications include: (i) estimating lithological zonations, (ii) providing direct constraints on hydrological parameters, (iii) incorporating geophysical data in hydrological inversions, and (iv) testing hydrological models and model predictions with geophysical models and time-lapse data. Complications in hydrogeophysical studies are often caused by non-unique relationships between geophysical models and data on the one hand, and hydrological properties and dependent variables on the other. Furthermore, the optimal target resolution in nonlinear inverse problems is difficult to define, such that error estimates of the resulting models and predictions are uncertain at best.

This special section will include method-oriented contributions that emphasize novel approaches for incorporating surface-based and crosshole geophysical data in quantitative hydrological flow and transport studies. Theoretical contributions and presentations based on field or laboratory experiments are most welcome. Research related to the integration or joint inversion of diverse data sets, model appraisal, ways to deal with space- and method-varying resolution, uncertainty estimation, and new hydrogeophysical rock physics models are also sought.

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Hydrograph shape and riverbed fine sediments on the Russian River

Authors: Rebecca Leonardson, James R. Hunt, William E. Dietrich, Deb Agarwal, Catharine van Ingen

Fine sediment such as silt fills the subsurface pore spaces in gravel riverbeds, reducing the flow of water between the river and the subsurface. This can have a number of consequences, including harming incubating fish eggs by cutting off the supply of dissolved oxygen and decreasing the water extraction rates in streambank filtration systems. Large storm events serve to clean the streambed by mobilizing gravel particles and washing away fines stored between them. However, there are a number of gaps in our understanding of the interactions between gravel, fine sediment, and time-varying river flow. Further complicating the picture is the erratic nature of sediment supply from upstream. Because of these knowledge gaps, there is no widely-accepted answer to the question: “how does hydrograph shape influence fine sediment dynamics in the gravel bed?” Several aspects of this question can be addressed through the analysis of measurements routinely taken on rivers by the United States Geological Survey (USGS). In particular, we propose that information about the entrainment of fine bed sediments can be extracted from high-frequency turbidity data, which is monitored to estimate suspended sediment concentration. To explore this bed sediment signal, a digital watershed has been created for the Russian River in Northern California, including six years of flow and sediment data reported at 15-minute intervals. The Russian River was chosen because of its very high suspended sediment load, the extensive set of monitoring data available from the USGS and other agencies, and the release of large pulses of water from a reservoir in the upper reaches of the watershed. A few days following large runoff events, the water level in the reservoir is rapidly lowered by a discharge of constant flow for a duration of 1-3 days. These pulses are easily distinguished from stormflows, due to the flashy hydrologic response of the basin. The dam releases serve as ideal experiments for studying fines entrainment because: 1) water is released at a constant flow, minimizing unsteady effects; 2) streamflow and turbidity are monitored at two sites, at 30 km and 120 km downstream of the dam, with an approximate travel time of 20 hours; and 3) the source of the sediment in suspension is limited to either the reservoir or the streambed. By computing mass fluxes as a function of time and location during dam releases, the following are estimated: · The maximum possible fines entrainment rate for a given volumetric streamflow on the Russian River · The storage of subsurface fines prior to the dam release · The time required to clean the bed of fines for a given streamflow and subsurface storage Because the storage of subsurface fines prior to the dam release is a function of the pattern of streamflow leading up to the release, this analysis also gives us a chance to study earlier, natural stormflows. Analysis indicates that the amount of fine sediment entrained is a function of both the size of the stormflow preceding the dam release and the amount of time that has passed since that flow occurred.

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Hydrological modeling and data assimilation system with the Land Information System

Authors: Sujay Kumar, Christa Peters-Lidard, Rolf Reichle, Randal Koster, Wade Crow, Xiwu Zhan, John Eylander, Paul Houser

The Land Information System is a hydrologic modeling system that integrates the use of several community land surface models, use of ground and satellite based observations, and high performance computing and data management tools to enable the assessment and prediction of hydrologic conditions at various spatial and temporal scales of interest. The LIS architecture is designed using advanced software engineering principles, enabling several interoperable features to incorporate new land surface models, observational data, land surface parameters, and meteorological forcings. The support for high performance computing has enabled high resolution modeling studies at previously unobtainable spatial scales. LIS has been coupled to the Weather Research and Forecasting (WRF) model, enabling a high-resolution land atmosphere system. Recently, the LIS framework has been enhanced by developing an interoperable extension for sequential data assimilation, thereby providing a comprehensive framework that can integrate data assimilation techniques, hydrologic models, observations and the required computing infrastructure. The capabilities are demonstrated using a suite of experiments that assimilate different sources of observational data into different land surface models to propagate observational information in space and time using assimilation algorithms of varying complexity. A number of experiments are conducted to assimilate surface soil moisture into different land surface models, to study the sensitivity of model parameterizations and physical representations on the efficiency of assimilation process. Experiments that demonstrate the assimilation of snow observations using different algorithms help in demonstrating the relative merits of each approaches. These results demonstrate the use of LIS framework as a valuable tool in the development, evaluation, and application of techniques for hydrological modeling

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Identification of Transport Parameters and an Uncertainty Analysis for a Physically Based Contaminant Transport Model with Spatially and Temporally Varying Recharge

Authors: Yong Yin, Jonathan F. Sykes, Stefano D. Normani

Contaminant transport parameter estimation and source characterization are crucial steps in the development of a physically based contaminant transport model. It is also an important prerequisite of the investigation of model uncertainty. Due to the ill-posed nature of the transport equations, inverse modeling and traditional gradient-based approaches can encounter difficulties in their application to real case studies. Heuristic search algorithms requiring extensive computing effort are deemed as promising approaches in the calibration of a contaminant transport model. High performance computing systems and parallel computing make this calibration process currently feasible. In this paper, the contaminant transport and source parameters were estimated and compared using optimization with a multi-start PEST algorithm and two heuristic search algorithms with these being a dynamically dimensioned search (DDS) and a parallelized micro genetic algorithm. The algorithms were implemented on the Shared Hierarchical Academic Research Computing Network (Sharcnet). The case study is located in Toms River, New Jersey, where a statistically significant childhood cancer cluster was found and could be related to the exposure to environmental contaminants. The Reich Farm site, where 4,500 drums of chemical wastes were dumped in 1971, is considered as a possible source of contaminants to the aquifer that serves a major well field for Toms River. A physically based transient groundwater flow model was developed to establish the historical relationship between the Reich Farm site and the municipal well field and to assist in the management and protection of the aquifer and well field. Groundwater flow from the Reich Farm Superfund site to the municipal well field for Toms River was modeled for a thirty-year time period using FRAC3DVS. In the model, spatially and temporally varying recharge, developed using the hydrologic model HELP3 in conjunction with GIS, was incorporated to account for water level fluctuations in observation wells resulted from seasonal and yearly variations of the recharge rate. The transient flow model was calibrated with the aid of approximately 9 years of head data from continuous well records as well as data collected over the entire period of the study using sampling at irregular periods. The contaminant transport model calibration results indicate that overall multi-start PEST performs best in terms of the final best objective function values with equal number of function evaluations, although the actual elapsed computer time for multi-start PEST is far less than the other two. Multi-start PEST was again employed to identify contaminant transport and source parameters under different averaging schemes of the spatially and temporally varying recharge. The estimated transverse dispersivity coefficients were demonstrated to be heavily affected by averaging of the recharge. Specifically, the estimated transverse dispersivity coefficients with spatially and temporally varying recharge were found to be significantly less than the dispersivity value calibrated with averaged, less physically based recharge values. Based on the multi-start PEST calibration results, a modified Latin Hypercube sampling approach accounting for correlation between parameters was employed to conduct an uncertainty analysis for contaminant concentration breakthrough at pumping wells.

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Identifying Dominant Transport Mechanisms Using Neural Networks

Authors: Ahmed E Hassan, Ahmed M. Tawfik, Hesham M Bekhit

Reactive contaminant transport in porous media is a very complicated process that is fraught with many uncertainties. When experimental breakthrough data are fitted to a model, it is essential to identify the dominant transport mechanisms in order to properly select the transport model. In this study we explore the use of trained neural networks to identify the appropriate transport model and provide the best fitting to experimental data. Neural networks models are successfully trained using five conceptually different transport models including linear and nonlinear, non-equilibrium sorption models and dual porosity models. A tool is developed linking five trained neural networks in such a way that given any experimental data set, the best model that can fit the data is identified and goodness-of-fit measures are provided. The tool is applied to a number of experimental data sets with good performance. The tool provides the advantage of saving enormous trial-and-error times that are usually associated with analyzing and fitting experimental breakthrough data.

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Imaging Biofilm Architecture in Porous Media

Authors: Danielle P. Jansik, Ryan T. Armstrong, Dorthe Wildenschild, Brian D. Wood

Current understanding of subsurface microbial biofilm formation and their impact on fluid hydrodynamics is limited by our ability to observe developed microbial colonies in their natural spatial arrangement. Biomass in porous media has mostly been observed in two dimensions, at the nanoscale, or at limited resolution in three dimensions; we are therefore lacking significant information about biofilm form. Three dimensional film arrangements can significantly alter pore flow velocities and overall mass transfer between the aqueous and biological phases. Further complicating this process is the potential for differences in biofilm density, arrangement, and distribution based on the geometry of porous media, fluid velocities and substrate availability. We are currently focusing efforts on resolving images using synchrotron based x-ray microtomography, imaging biofilms without disturbing their natural spatial arrangement has been a challenging task, as dopants typically dissolved in water easily diffuse into biomass. By adding colloidal silver to the solution we have been able to differentiate between the biomass filled pore space and fluid filled pore space. At this point, data collected has provided qualitative information about structures of biomass and how they may alter the physical properties of the porous media. We believe this approach shows potential for future quantification of biofilm form. Ultimately, by quantifying form we will gain a greater understanding of how changes in physical parameters may impact the rate at which microbes degrade contaminants, and therefore alter the effectiveness of bioremediation.

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Impact of Changing Climate on Water Resources

Authors: Namrata Batra, Praveen Kumar, Yi-Chen E. Yang, Hyun Il Choi, Praveen Kumar, Ximing Cai, Charlotte De Fraiture

(1,3,4) Hydrosystems Laboratory, Department of Civil and Environmental Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA.

(2)Center for Atmospheric Science, Illinois State Water Survey, University of Illinois, Champaign, Illinois, USA.

(3)International Water Management Institute, Colombo, Sri Lanka.

Climate change varies from region to region. This variation is driven by the uneven distribution of solar heating, land cover changes, the individual responses of the atmosphere, oceans, land surface and the underlying complex interactions, the physical characteristics of the regions, etc (AR4, IPCC 2007). With advances in modeling and understanding of the physical processes of the climate system, more reliable regional climate change projections are now available. Hydrologic models have not yet been extensively explored for their ability to capture the impact of changing climate and their subsequent influence on water resources. We seek to achieve long term sustainability of water resources in different regions of the world using an advanced hydrologic model and data sources.

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Impact of groundwater pumping on near-river hydrology

Authors: Yingqi Zhang, Michael B. Kowalsky, Stefan Finsterle , Susan Hubbard

In this study, we develop a model to better understand stream-groundwater interactions at a site adjacent to the Russian River in Northern California where high-capacity collector wells extract groundwater from an aquifer underlying the streambed. Despite the seasonal use of a rubber dam to increase the upstream water level and thus increase recharge to the aquifer, an unsaturated zone occasionally develops beneath the streambed, reducing pumping capacity and altering chemical and biological transformations, which may affect drinking water quality. The modeled area encompasses a relatively large region, including three collector wells and an array of monitoring wells for which temperature and pressure data are available, and two infiltration ponds. To accurately simulate the flow of air and water during development of the unsaturated zone beneath the river bed, the multiphase flow simulator TOUGH2 is used. iTOUGH2, a code that provides inverse capabilities for TOUGH2, is used to estimate the most relevant model parameters based on data collected at the site during 2006. The overall objectives of this study are 1) to gain a better understanding of the stream-groundwater interaction; 2) to investigate how major hydrological factors (e.g., permeability contrast between the streambed and aquifer) affect the unsaturated zone development beneath the streambed; 3) to examine how the development of the unsaturated zone responds to the river stage, as a result of the raising or lowering of the inflatable dam; 4) to evaluate the effects on the pumping capacity as a result of changes in the hydrological conditions of the streambed when there is a change in the operation of the inflatable dam; and 5) to provide a basis for the subsequent joint inversion of hydrogeological and geophysical data, which are being collected in ongoing work. The results will help optimize management of the inflatable dam and groundwater pumping activities in this region.

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Impact of Pore-scale Spatial Heterogeneity on Macroscopic Solute Dispersion

Authors: Branko Bijeljic, Martin J. Blunt

Understanding solute transport in porous media is of central importance in the design of remediation schemes for contaminated groundwater, radioactive waste disposal and tracer studies in oil recovery. Solute transport in a porous medium is characterized by the interplay of advection and diffusion (described by Peclet number, Pe) that cause spreading of solute particles. This spreading is traditionally described by dispersion coefficients, D, defined by s2 = 2Dt, where s2 is the variance of the solute position and t is the time. In the asymptotic limit D is constant and can be used in an averaged advection-dispersion equation. However, it is highly important to recognize that, until the velocity field is fully sampled, the particle transport is non-Gaussian and D possesses temporal or spatial variation. Transport properties in real systems are difficult to predict because they are geologically heterogeneous from the pore scale upwards. In order to study the impact of spatial heterogeneity on macroscopic solute dispersion we use pore-scale model with the geometry and topology based on the networks extracted from the micro CT images of a number of sandstone and carbonate core samples. We study spatial and temporal probability density functions of tracer particles by using a Lagrangian pore-scale network model that incorporates flow and diffusion in three-dimensional irregular network lattices. The impact of heterogeneity is presented in both pre-asymptotic and asymptotic dispersion regime by probability density functions and dispersion coefficients, for a range of Pe. We discriminate the onsets of the restricted diffusion, transition, power-law and mechanical dispersion regimes for the sandstones and carbonates studied. Moreover, we show that the length traveled by solute plumes before Gaussian behaviour is reached increases with an increase in heterogeneity and/or Pe. This opens up the question on the nature of dispersion in natural systems where the heterogeneities at the larger scales will significantly increase the range of velocities in the reservoir, thus significantly delaying the asymptotic approach to Gaussian behaviour. As a consequence, the asymptotic behaviour might not be reached at the field scale.

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Impact of Uncertainty Estimation on Early Assessment of Technology Options in Contaminated Land Management

Authors: Albert Yeboah-Forson, Michael Finkel, Ursula S. McKnight

Large-scale sites with contaminated land and groundwater constitute a complex system with numerous interacting processes that impact not only the environment but also major areas of society such as human health, the economy and the environment. Due to the scale and complexity of these sites, there are usually a great number of possible management options that could be considered. Since a detailed investigation of all these options is not economically feasible, a streamlining of the planning and decision process is a mandatory requirement, beginning with an early selection of promising management options based on a preliminary assessment. In this context, the knowledge of uncertainties can help to gear future, more detailed investigations towards favored options and thereby streamline the management process. In this study the results of an investigation carried out to determine and rank parameters with respect to their relative importance to the cost–efficiency analysis of remediation options are presented. Monte-Carlo simulations using the assessment model CARO-plus were used to analyze the effect of uncertain parameters in the context of LNAPL groundwater contamination scenarios. The results indicate that the initial contaminated mass and the groundwater recharge are the most critical parameters of concern. The cost of remediation using a pump and treat system (PTS) was shown to be influenced by both the uncertainty in site specific parameters, as well as uncertainty inherent in the PTS technology such as overpumping factor and pump efficiency.

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Implementation of reaction-induced multicomponent gas transport into a vadose zone reactive transport model

Authors: S. Molins, K.U. Mayer

The consumption or production of gases by biogeochemical reactions in the vadose zone can drive significant diffusive and advective gas fluxes. To simulate reaction induced gas transport, multicomponent gas diffusion and advection have been implemented into a variably saturated reactive transport model. The model has been used to assess the contributions of various gas transport processes in systems of environmental relevance such as landfill soil covers, mine tailings, and an oil contaminated site. In the implementation of the model, gas transport is implicitly substituted in the mass balance equation. Two approaches to incorporate the gas flux terms in the mass balance equations are considered. In the first formulation, advective and diffusive contributions are calculated separately for each component. Darcy's law is used for advection, while the Dusty Gas Model equations (DGM) are used for diffusion. In the second formulation, the Dusty Gas Model equations are written in terms of net fluxes, which include both advective and diffusive fluxes. The net contribution is then added to the mass balance equation of each component. In this approach, Darcy's law only appears explicitly in the Knudsen diffusion term. In this work, we show that both formulations are equivalent, and we compare the numerical efficiency of each approach for the simulation of gas transport in a number of systems of interest. In this context, we analyze the numerical burden associated with the calculation of advective and diffusive contributions.

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Implicit Sub-timing in Flow and Transport Simulations

Authors: Sorab Panday, S. Murty Bhallamudi, Edward Sudicky

Simulations of flow and transport that utilize an implicit time marching procedure require that a time-step size be the same throughout the solution domain. This can lead to an over-discretization in the temporal domain at several locations within each time step of a simulation. A sub-time stepping procedure is described within the framework of a fully implicit formulation, which allows for use of nested smaller time-step sizes in portions of a domain where activity and interest is high, with larger time-step sizes in other locations. Effects of sub-timing on the matrix structure and on computational gain are discussed. The methodology is demonstrated with proof-of-concept problems and applied in an adaptive manner to a transport situation where the local Courant Number needs to be controlled and to a large-scale fracture flow and transport simulation case.

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Improved accuracy and efficiency for the simulation of strong feedback of chemistry on hydrodynamics based on operator splitting

Authors: Vincent Lagneau, Jan van der Lee

Reactive transport is a highly non-linear problem that requires the most efficient algorithms in order to reach an accurate solution. Two classes of formulations are usually found in the literature: the global implicit approach or direct substitution on the one hand, the operator splitting method on the other hand. Operator splitting appears to be an accurate approach, provided that the solution is iteratively improved for each timestep. Iterative improvement is particularly important in the case of feedback of dissolution or precipitation reactions on hydrodynamic flow and transport, commonly referred to as the variable porosity case. An analytical solution of a diffusive problem has been developed to test the accuracy of the numerical model HYTEC. An iterative resolution of variable porosity cases is often CPU consuming, especially if full clogging is approached which leads to a very stiff system and therefore small timesteps. Efficiency is therefore a key-issue if we want to apply reactive transport models to large scales and real-world problems. Here we propose an efficient estimator/corrector method based on the physico-chemical behavior of the system that allows to reach convergence faster and to reduce stiffness. The efficiency improvement is significant as illustrated at the hand of an example of carbonation of a cement paste, a well-known problem that leads to complete clogging of the interface layer.

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Improving the Computational Efficiency of a Multicomponent Reactive Transport Simulator

Authors: Vicky L. Freedman, Steven B. Yabusaki, Matt Rosing, Andy L. Ward

A significant issue facing the Department of Energy (DOE) is the behavior of liquid wastes that react and alter chemical conditions as they migrate through naturally complex subsurface materials. The orders-of-magnitude range in values and multiple scales of spatial variation in typical soil parameters are important to the accurate simulation of contaminant behavior. At an experimental vadose zone test site in the Hanford 200 East Area, hydrogeological properties at the cm-scale were characterized using in-situ measurements, and statistical correlation was used to estimate the cation exchange capacity. Three-dimensional reactive transport simulations for an experimental release of strontium and magnesium were performed at 2.5 cm spatial resolution to identify the impact of multiscale property variability on the behavior of strontium in the vadose zone. The CRUNCH simulator that was used for this application is designed to model multicomponent, multi-dimensional reactive transport in porous media. The 10-year simulation of multicomponent ion exchange includes reactions among 11 primary chemical components, 30 secondary species, 5 ion exchange species, and 6 minerals throughout the 14.224 m x 13.4112 m x 12.827 m problem domain that is represented by a 560 x 528 x 505 cartesian grid (149,318,400 grid cells). Several improvements were made to the parallel version of CRUNCH to improve the peak aggregate theoretical performance on the MSCF NWMPP2 cluster simulating the three-dimensional infiltration of a strontium-magnesium solution into the highly-resolved three-dimensional unsaturated porous media. These improvements included vectorization of the chemistry routines in the operator splitting solution procedure and specializing the code for the specific application. The resulting code, when run on 1848 processors (~ the entire NWMPP2 cluster) for the roughly 150M grid cell problem domain, yielded an improvement to roughly 20% of peak performance across the entire machine within the time loop. An even larger efficiency, and faster time-to-solution, can be expected for calculations of the same size on a smaller number of processors.

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Incorporating substrate bioavailability in reactive transport models for biodegradation processes

Authors: Martin Thullner

Reactive transport models have emerged as an essential diagnostic tool for the quantitative analysis of the biogeochemical functioning of complex subsurface environments and, in particular, for the assessment of the fate of contaminants and the interpretation of the distributions of reactive chemical species. Reactive transport model applications range from contaminated aquifers to aquatic sediments in freshwater and marine environments. Thus, the assessment of contaminated sites and their remediation is often based on the results of reactive transport simulations providing the most comprehensive analysis. Nonetheless, reactive transport modeling of subsurface environments still faces many challenges, including the development of realistic model representations of microbial reaction kinetics. Currently, many reactive transport approaches are based on empirical or simplifying relations describing microbially controlled reaction rates. Although simple modeling studies can be beneficial for reproducing measured data sets or calculating mass balances, an oversimplified description of processes can lead to error compensation and obtained parameters are effective parameters for a given site at a given time period, without predictive power for other sites or time periods. Furthermore, concepts linking such effective parameters to measured laboratory data on microbial kinetics are not well developed. Thus, there remains a need for further development of more general, process-based modeling concepts to represent microbially mediated reactive processes. In particular, these concepts need to consider that the in situ (degradation) activity of microorganisms in the subsurface depends on the bioavailability of growth substrates, for example, organic carbon, TEAs and nutrients. However, total macroscopic concentrations are not necessarily a good measure of the bioavailability of a chemical substrate. This might be due to the fact that the substrate is not in a chemical or physical state that allows direct microbial utilization. In other cases, bioavailability may be limited because the substrates are not in the same location as the microorganisms. The concentrations determined experimentally only represent an average over the sampling scale and the concentration of a dissolved chemical substrate in the immediate vicinity of a metabolically active cell may differ significantly from the average concentration in the porous medium. The consumption rate of the substrate then depends on the transfer rate of the substrate from the bulk pore solution to the cell. Bioavailability issues are a challenge for reactive transport modeling at any scale. This presentation exemplifies existing approaches and discusses some novel approaches to include bioavailability aspects into reactive transport modeling concepts.

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Incorporating transport processes into a coupled model of surface and subsurface interactions

Authors: Sylvain Weill, Annamaria Mazzia, Claudio Paniconi, Mario Putti

In hydrology, ecology, and environmental management and protection there is increasing attention paid to how water and solutes are exchanged between the atmosphere, the land surface (including open water bodies), and the subsurface (soils and aquifers). In addition, the transfer and transport of contaminants and other solutes is intricately linked to water dynamics. Appropriate mathematical equations governing surface and subsurface processes of water flow and solute transport exist but can be very difficult to solve, owing to nonlinearities, sharp propagation fronts, heterogeneities, and other factors. Further complexity is added when interactions, or coupling, across the land surface interface are taken into account. In this work we consider the implications of these complexities on appropriate numerical schemes for solving flow and transport in a coupled surface--subsurface model. Such a model needs to balance accuracy and efficiency on many fronts: linearization schemes (in particular for the strongly nonlinear Richards equation); adaptive and nested time stepping (that considers also the different characteristic scales of surface and subsurface dynamics); resolution of advection-dominated transport phenomena; calculation of the velocities and discharges that are passed from the flow module to the transport solver; and representation of the land surface boundary condition and of the exchange terms for solutes and water across this interface. A prototype model will be presented that is based on the three-dimensional Richards equation for flow in variably saturated porous media, a path-based (rill flow) diffusion wave approximation to the Saint-Venant equations for surface dynamics on hillslopes and in stream channels, and the classical advection-dispersion-reaction equation with first-order mass transfer. Numerical solution schemes include mixed finite elements for discretization of the flow equations and coupled finite element-finite volumes for the transport equation.

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Influence of soil structure on estimation of effective parameters in the unsaturated zone

Authors: Milos Vasin, Insa Neuweiler, Peter Lehmann, Rene Hassanein, Anders Kaestner, Eberhard Lehmann

Heterogeneity of the soil parameters effects flow in the unsaturated zone. When the flow in the unsaturated zone is modelled, the heterogeneity can not be resolved in detail. Therefore, simplified (upscaled) models have to be derived, which allow us to handle the complexity of the processes, but still capture the influence of the heterogeneities as far as possible. The main goal of this study was to assess the potential of predicting flow with an upscaled models and to analyse influence of the structure on the effective model parameters. To this end, multi-step drainage experiments in two heterogeneously packed sand columns (10x10x20 cm3) have been performed. Two different packing structures were generated using sand cubes of 1x1x1 cm3 of two different sand types. The heterogeneous structures of the columns can be considered as two opposing extremes. The first column was packed with a random arrangement of the two sand types with a column-spanning connected cluster for both materials. The second column was packed with a periodic pattern of coarse sand inclusions in a fine sand background, having a clearly defined unit cell. Beside the outflow, the depth averaged (2D) spatial distribution of the water content in the columns was monitored during the whole multi-step outflow experiment using neutron radiography. 3D water content was measured at steady state by neutron tomography. The experimental results are compared to model predictions of an upscaled model derived with homogenization theory. Effective parameters for upscaled models were first derived with a set of parameters predicted from the pore scale structure of the two individual sand types. The predictions with these parameters will be discussed in the talk in order to assess the potential of predicting soil parameters from pore scale properties. Additionally, the hydraulic parameters of both sands were identified by fitting the model predictions to the measured outflow curves. The different column structures showed a significant effect on water retention and the effective retention function, as water was trapped in the coarse-sand inclusions of the periodic structure. We included this effect of trapping in the effective retention function of the upscaled model with an apparent air entry pressure. Contrary to the retention, the different packing structures had no large effect on the dynamic behaviour of outflow. The upscaled models predicted the movement of the averaged water content in the two columns well, also in the randomly packed column where the assumptions made for the upscaled model are not strictly met.

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Integrating GIS Web applications with OLAP and RDBMS

Authors: Matt Rodriguez

Several online GIS applications are being developed within the CUAHSI Hydrologic Information System (HIS) project, to enable map-based discovery and access to multiple observations data repositories assembled at federal agencies, and by individual researchers. The online applications such as the Data Access System for Hydrology (DASH) and Hydroseek rely on observations data catalogs that follow a uniform relational schema known as CUAHSI Observations Data Model (ODM). The currently available catalogs describe several nation-wide data repositories that are important for hydrologists, including USGS NWIS, EPA STORET, USDA's SNOTEL, and NCDC's ASOS. The catalogs provide a summary of information regarding the amount and type of data available for each data collection, and extensive metadata describing measurement stations, observed properties, periods of record, processing methods, etc. The catalogs are stored in MS SQL Server 2005, and accessed from the GIS applications either directly, or via CUAHSI WaterOneFlow services. The current system supports efficient browsing and querying of observations data by stations. However, summary data availability requests in such a system may be fairly slow, especially with more data being registered. OLAP is a multidimensional data model that has great performance for a certain class of queries. This class contains queries that are useful at summarizing a data collection along different temporal and spatial dimensions. An example query where OLAP performance is superior to a relational DBMS is finding total number of stream gage measurements in a given state (county, HUC, or another area or group of areas) for a given year, or another temporal unit. Both spatial and temporal dimensions, and other dimensions included in the OLAP cube, can be organized hierarchically which gives considerable flexibility in formulating catalog queries. OLAP has better performance than a RDBMS for these kinds of queries because of how the data is indexed and aggregated in the OLAP system. OLAP technology can be used to dynamically generate series catalog information thus enabling GIS web applications to scale as the size of hydrological collections grows. The ability of the web application to formulate catalog queries and the performance of the OLAP system provide the interactivity required for the Web GIS application. This conference presentation will include a discussion of OLAP integration into CUAHSI HIS catalog management to support the central HIS server at SDSC. In particular, we will focus on embedding OLAP cubes for large federal repositories, as well as custom OLAP cubes integrating watershed data from multiple sources, in the HIS server and DASH, and present statistics on the query performance improvement.

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Integrated Modelling of Surface-subsurface Flow Systems over Multiple Scales

Author: E.A. Sudicky

Over the past several years, increasing attention has been directed towards understanding flow and solute transport processes occurring at the interface between surface water and groundwater, and a variety of numerical strategies have been proposed to couple these processes in a holistic, physically-based modelling framework. Management of watersheds and ecosystems requires such numerical models that can simulate surface and subsurface water flow and solute transport. This lecture will present an overview of the capabilities and recent developments of the HydroGeoSphere model together with several applications. HydroGeoSphere is a fully-coupled 3D model designed to simulate water flow and advective-dispersive solute and heat transport on the 2D land surface and in the 3D subsurface under variably-saturated conditions. Full coupling of the surface and subsurface flow regimes is accomplished implicitly by simultaneously solving one system of non-linear discrete equations describing flow and transport in both flow regimes, as well as the water and solute fluxes between continua. Other model features are the inclusion of heterogeneous material properties in all regimes, discrete fractures, dual-permeability flow and transport, canopy interception and evapotranspiration governed by plant and climatic conditions, as well as density-dependent flow and transport in the subsurface. The model capabilities and main features are demonstrated with several 3D numerical simulations performed for catchments of various scales. The examples range from the scale of an intensively-monitored rainfall-runoff-tracer experiment (~ 2000 m2), to a regional-scale watershed of about 300 km2, to the continental scale that comprises a simulation of the impact of the Wisconsinian glaciation on groundwater flow system and groundwater age evolution (-120 k-year to present) over the entire Canadian land mass. For the latter example, the University of Toronto's Glacial Systems Model is used to drive HydroGeoSphere, and includes the impact of ice sheet loading and unloading, isostasy, permafrost formation and thawing, and recharge from subglacial meltwater production. The simulations highlight the difficulties and challenges for representing water flow and solute transport in complex natural systems, and stress the advantage of using a process-based model such as HydroGeoSphere for prediction of current and future water management scenarios.

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Integration Of Multi-Scale Networks Of Heterogeneous Porous Media And Their Multi-Phase Flow Prediction

Authors: Kejian Wu, Andrey RYAZANOV, Zeyun Jiang, Rink van Dijke, Ken Sorbie, Gary Couples

ABSTRACT Current methods of hydrocarbon reservoir and aquifer flow performance use continuum-scale numerical simulations which depend upon quantification of the multi-phase flow characteristics for each grid block in the simulation. The ultimate control on multi-scale flow occurs at the pore scale, since no matter how large the scale of an oil reservoir is, the injected fluid (water or gas) will displace the oil pore by pore. Highly irregular grain shapes and sizes result in complex pore shapes, with size distributions that may vary over 5 orders of magnitude, from micropores with pore throats of much less m to substantial macrospore systems. The existence of such multi-scaleμthan 1 and highly complex 3D networks of connected pores makes multi-phase flow behaviour difficult to predict. We introduce a new method of integrating multi-scale pore systems. A stochastic 3D pore space reconstruction model is employed that uses different scale thin section images as its main input. The approach involves a third-order Markov mesh that creates the reconstruction in a single scan, thus overcoming the computational issues normally associated with Markov chain methods. The technique is capable of generating a realistic “pore architecture model” (PAM) of a fairly heterogeneous rock samples at a given scale. PAMs, or tomography models, serve as input for another suite of analysis techniques that we call pore analysis tools (PATs) to obtain geometrical and topological (G-T) characteristics (i.e. size and shape, as well as connectivity and tortuosity). Based on PATs, we are able to extract well-characterized G-T network models that are used for simulating two- and three-phase fluid flow. Extracted networks from different scaled porous rock images are integrated into an idealised multi-scale nested network to predict flow properties of multi-scale heterogeneous porous media. We apply this technique to integrate the submicron and micron scales in the first instance, for which the different scale PAMs have different pore size distributions and the resulting pore networks have distinct flow properties.

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Intelligent Analysis of Prediction Uncertainty

Authors: Mary C. Hill, US Geological Survey, and Ming Ye, Florida State University

Meaningful evaluations of prediction uncertainty require methods with the following characteristics:

- They need to be computationally tractable for the long execution times characteristically needed to represent realistically natural hydrologic systems.
- They need to clearly indicate what aspects of the data and model construction are dominating the calculated measures of uncertainty.
- They need to indicate how to reduce uncertainty, by collecting more parameter measurements and observation data.
- They need to account for different types of error, including errors in the data used for model development, errors in estimated parameters, and errors in the conceptual model.
- They need to be generally applicable, and not limited to rarely satisfied conditions and assumptions.
- The methods and results need to be statistically valid and make sense from the perspective of common sense.
- They need to adequately measure prediction uncertainty, and the measures should be understandable to nonspecialists, such as policy makers.

Currently, most scientific advances focus on some part of these issues. This session seeks to bring scientists together to present their contributions on sensitivity analysis, parameter estimation, and uncertainty assessment, and to develop a vision of how the methods we are all developing can contribute to a truly intelligent way of analyzing prediction uncertainty.

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Interface integral BEM for solving seepage problems in nonhomogeneous media

Authors: Xiao-Wei GAO, Jing WANG, Kai YANG

In this paper, a simple boundary element method, called IIBEM, is presented for solving seepage problems consisting of different materials characterized by different hydraulic transmissivities. The main feature of the IIBEM is that a multiple material problem can be solved by using a single boundary integral equation. The effect of nonhomogeneity between adjacent materials is reflected by an interface integral appearing in the basic boundary integral equation, which includes the material property difference between two adjacent materials. Comparing to the conventional multi-domain boundary element method (MDBEM) [1, 2], the presented method is more efficient in computational time, data preparing, and program coding. Numerical examples regarding underground water flows through porous media are given to demonstrate the potential of the presented method. References [1] Gao XW. Three-step multi-domain BEM solver for nonhomogeneous material problems. Engineering Analysis with Boundary Elements 2007; 31: 965–973. [2] Kane JH, Kashava Kumar BL, Saigal S. An arbitrary condensing, noncondensing solution strategy for large scale, multi-zone boundary element analysis. Comput. Methods Appl. Mech. Eng. 1990; 79: 219-244. [3] Divo EA, Kassab AJ. Boundary Element methods for Heat Conduction: With Applications in Non-homogeneous Media. WIT Press: Southampton, 2003.

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Inverse analysis of temporal high-frequency pressure and water-supply pumping data to identify aquifer properties

Authors: Velimir Vesselinov, Dylan Harp

Water-supply production at wellfields is frequently characterized by substantial temporal and spatial variability. In general, different production wells are operated and rested at different times and the total production is controlled by demand which peaks in the summer and decreases in the winter. During the wellfield operation high-frequency water-level data are also commonly collected in the production and nearby observation wells. In a way, such a scenario can be viewed as a single prolonged and data-intensive pumping test which includes multiple pumping and observation wells. All these data can be interpreted simultaneously using simple analytical techniques as well as complicated 3D numerical models. The analytical techniques facilitate the initial screening of the data and the identification of correlations between the pumping and water-level variability. The numerical models can be applied to characterize the spatial heterogeneity of the tested flow medium. Here we discuss the high-frequency pressure and water-supply pumping data acquired during the water-supply production near the Los Alamos National Laboratory and their interpretation by means of analytical and numerical techniques.

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Inverse microbial and geochemical reactive transport models

Authors: Javier SAmper, Changbing Yang, Javier SAmper

Microbial processes play a major role in controlling geochemical conditions in subsurface systems. Various laboratory and in situ experiments have been performed to evaluate the relevance of microbial processes and derive key microbial parameters. Such experiments are often interpreted in a subjective manner by trial-and-error curve fitting. A numerical model for the inverse problem of coupled flow, reactive solute transport, geochemical and microbial processes is presented here which overcomes the limitations of trial-and-error methods by making data interpretation in a systematic, objective, and efficient manner. It extends the capabilities of existing inverse models which deal mostly with flow and chemically-reactive solute transport. Our inverse model relies on the microbial reactive transport model of Zhang (2001) and Samper et al. (2006a) and improves the inverse reactive transport model of Dai and Samper (2004) by allowing the simultaneous estimation of geochemical and microbial parameters. The inverse model has been implemented in a finite element code, INVERSE-BIOCORE2D and its capabilities have been verified and tested with a synthetic experiment involving equilibrium speciation, kinetic sorption/desorption and kinetic biodegradation reactions. Model results indicate that both chemical and microbial parameters can be estimated accurately for error-free data. Estimation errors of microbial parameters are larger than those of kinetic sorption parameters and generally increase with increasing standard deviation of data noise. Estimation error of yield coefficient is the smallest among all microbial parameter and which does not depend on data noise. The inverse model has been used also to estimate microbial parameters of DOC aerobic respiration responsible for oxygen consumption at the REX in situ experiment. Estimates of microbial parameters are found to be within the range of reported values and have small estimation errors.

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Investigating empirical equations of determining time of concentration of flood

Authors: Baharak Motamedvaziri

Time parameters are used mostly in hydrologic and hydrolic models. The most often used time parameter in hydrology is time of concentration. Time of Concentration is the time required for a particle of water to travel from the hydrologically most distant point in the watershed to outlet or designing point. Time of Concentration is used for designing spillway, estimating flood volume, preparing flood hydrograph and many other hydrologic analysis. many methods (empirical equations) are available for estimating time of concentration. the aim of this research is selecting the best method(s) for estimating time of concentration in the studied basin. To achieve the said aim , a field method based on measurement of travel time by salt solution is used. In order to select the best method(s) for estimating time of concentration in the basin, the defference between values obtained by using these methods and the field method are determined. Results of this research show that In steep area, SCS Lag method is the best for estimating time of concentration. In this area Ventura, Gianduti, Passini, and Carter methods provide a fairly good estimate of time of concentration. In flat area, Chow, Kirpich, Basoo, and California methods provide a fairly good estimate.

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Investigation of the IMpacts of Climate Change on Crop Productivity and Drought Events

Authors: Greg Husak, Chris Funk, Mike Dettinger, Diego Pedreros, James Verdin

Recent research by scientists at Scripps has produced high quality high resolution precipitation time-series for the 21st century based on the GFDL and PCM models. This study analyzes this data with two common drought monitoring tools: Standardized Precipitation Index (SPI) and the crop Water Requirement Satisfaction Index (WRSI) imagery. SPI expresses precipitation accumulations in terms of the probability of exceedance based on a standard normal distribution. This reflects the significance of an event more completely than the anomaly or percent of normal measurement. Another positive aspect of the SPI is that the likelihood of the measurement does not change in time or space, unlike anomaly or percent of normal measures. Setting thresholds of SPI to define extreme rainfall events, we look at changes in the likelihood of these extreme events in downscaled rainfall. We also investigate how these changing frequencies may affect crop conditions. WRSI evaluates crop-specific water stress based on a phenologically augmented soil water balance. Analysis of the WRSI time-series focuses on potential shifts in the frequency of water stress for several crops. This information reveals the impacts of potential climate change on crop productivity for different regions. The project will also evaluate historical relationships between observed precipitation, temperature and potential evapotranspiration (PET), and produce 21st century projections of PET based on these relationships. These PET fields will be incorporated in the WRSI runs and the impacts evaluated. This project leverages consistent time series of precipitation and temperature fields that extend far enough in history to create meaningful probability distributions of events, and far enough into the future to make reasonable forecasts about the likelihood of significant events. Framing the future conditions in terms of the frequency of extreme events, especially drought, and the affects on crop health connects potentially changing conditions to two key impacts. These impacts serve as indicators for regions which may be most affected by climate change in the coming century.

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Iterative Multiscale Finite-Volume Method

Authors: Hadi Hajibeygi, Marc Andre Hesse, Giuseppe Bonfigli, Patrick Jenny

Natural porous media are typically governed by highly heterogeneous coefficients with complex spatial distribution. While current advances in characterization and data integration provide increasingly detailed descriptions of the subsurface, classical simulation techniques lack the capability to honor all these fine-scale structures. The multiscale finite-volume (MSFV) method deals with this resolution gap and aims to reduce the computational complexity of the problem based on local numerical solutions of the fine-scale problem. Therefore, its quality depends on the localization assumptions, i.e. the assumed boundary conditions required to solve the localized problems. Although the MSFV proved to be very accurate for a broad range of test cases, the errors resulting from the localization assumptions can be considerable, especially in the presence of large (with respect to the coarse cells) coherent structures with high permeability contrast, e.g. nearly impermeable shale layers. Moreover, the accuracy of the method suffers in the presence of highly anisotropic-heterogeneous media. For further improvements, global information can be employed to improve the boundary conditions of the local problems. In this paper, we present an iterative multiscale finite-volume (i-MSFV) algorithm for stiff elliptic problems. The basic idea of the new method consists in successively improving the localization assumption by employing the global approximate multiscale solution from the previous iteration. Numerical convergence of the method is verified for different test cases ranging from solving the standard Poisson equation to highly heterogeneous, anisotropic Elliptic problems and it is demonstrated that it allows to effectively reduce the error by only a few iterations. While the i-MSFV method can still be employed as a typical multiscale method (without iteration it is identical to the MSFV method), it can also be used as an efficient linear solver. Moreover, since it is possible to construct a conservative fine-scale velocity field at each iteration level, the i-MSFV method can be operated anywhere between these two extreme modes. Finally, to demonstrate the efficiency of the method for multiphase transport in porous media, it is shown that it is sufficient to apply the iterative procedure only frequently; i.e. not every time step. This result is crucial, since it tells us that the overall efficiency of the i-MSFV algorithm is almost as good as that of the original MSFV method. At the same time, even the solutions of the most challenging cases are significantly improved.

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Joint inversion for hydrogeophysical facies zonation through level set methods

Authors: Michael Cardiff, Peter Kitanidis

Geophysical data holds the promise of enabling detailed aquifer characterization through the use of techniques that, relative to most hydrologic characterization techniques, are cheap and fast to implement. Geophysical methods - including seismic, GPR, and ERT methods - are especially useful in areas where large parameter variability is present, as these datasets can help to more tightly constrain geologic facies distributions or parameter "zones". The key problem in utilizing many geophysical datasets is that the data are only indirectly dependent on hydrologic parameters of interest, such as hydraulic conductivity or porosity. Two main approaches have been implemented for integrating geophysical data. The first approach, a "petrophysical relation" approach, assumes that geophysical parameter values can be related to hydrologic parameter values through a unique relation. The second approach, a "zonation" approach, assumes that geophysical parameters can be used to produce a map of geologic zones, and subsequently assigns hydrologic parameter values (usually uniform) to those zones using additional data. Both approaches suffer from significant disadvantages. Petrophysical relation approaches are difficult to apply when non-unique relationships between hydrologic and geophysical parameters exist. Conversely, zonation approaches allow non-unique parameter relationships but generally under-emphasize the zonation information conveyed by hydrologic data. In this work, we present results on the use of level sets for lithologic zonation, and extend the use of level sets to joint inversion of hydrologic and geophysical data. This joint inversion strategy does not require unique petrophysical relations and allows several datasets to drive the location of facies boundaries. Originally developed for modeling the complex evolution of fluid interfaces, level set methods provide a flexible way to represent arbitrarily complex geologic facies boundaries within an inverse problem. The optimization of zone boundaries through the level set method, while nonlinear, can generally be solved via gradient searches. During this presentation, we review the basic theory behind optimizing facies boundaries with level sets. We show performance on example inverse imaging problems, emphasizing the flexibility of this method to represent zones of any shape, size, or number. While traditionally level sets are used to differentiate between only two materials (i.e., a Boolean field), we show how they may also be used to represent an arbitrary number of facies. We demonstrate the ability of our level set method to recover zone boundaries from sparse, noisy data. Comparisons are made between the level set method and other zonation strategies, such as image thresholding and Voronoi cell optimization. Finally, we discuss how level sets may be used in joint inversion where both hydrologic and geophysical data deform and improve zone boundaries. Throughout our work we adopt a Bayesian approach which allows us to logically integrate prior information, estimate parameter uncertainty, and generate conditional realizations of the imaged domain.

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Kinetics of conjugative gene transfer on surfaces in granular porous media.

Authors: A. Massoudieh, T. R. Ginn, K. E. Nelson, A. Mathew, E. Lambertini, C. Crain, T. Barkouki, P. L\\\'Amoreaux, F. J. Loge

The transfer of genetic material among bacteria in the environment can occur both in the planktonic and attached state. Given the propensity of organisms to exist in sessile microbial communities in oligotrophic conditions, and that such conditions typify the subsurface, we explore via modeling and experiments the horizontal transfer of genes by conjugation in granular porous media. Rates of attachment/detachment and conjugation among surface-associated E. coli were obtained from empirical data collected using scanning confocal laser microscopy with glass beads packed within a microflow chamber. The mathematics so far used to describe the kinetics of conjugation are developed largely from experimental observations of planktonic gene transfer, and are absent of lags or plasmid stability that appear experimentally. We develop a model for bacterial filtration, and gene transfer in the attached state, for the early stages of biofilm formation. We include attachment kinetics described using the filtration theory approach of Nelson and Ginn (2005) with motility of E.coli described according to Biondi et al. (1998).

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Lattice-Boltzmann Simulations Of The P_{c} − S − a_{nw} Relationship

Authors: Mark L. Porter, Dorthe Wildenschild, Marcel G. Schaap

Capillary pressure plays an important role in multiphase flow through porous media. At the microscale, capillary pressure is defined by Laplace's law, which takes into account interfacial phenomena such as surface tension, interfacial curvature and the contact angle. However, at the macroscale, capillary pressure is taken to be a function of the wetting phase saturation alone and the pressures are measured separately in each phase, typically outside the porous medium. It has been hypothesized that in addition to saturation, capillary pressure should be a function of interfacial area per volume. In this study we compare interfacial areas obtained from microtomographic image data and lattice-Boltzmann simulations for drainage and imbibition processes. It is shown that there is good agreement between the measured and simulated capillary pressure curves. In addition, there is agreement between the interfacial area estimates for drainage. The interfacial area for imbibition is higher in the simulations than in the experiments. Image analysis indicates that during imbibition there is substantially more flow via films in the lattice-Boltzmann simulations than in the experiments, which may explain the higher interfacial areas. Scanning curves for imbibition and drainage were also simulated and a surface was fit to the capillary pressure - saturation interfacial area data. The surface indicates that the additional dependence of capillary pressure on interfacial area may provide insights into the hysteretic nature of the capillary pressure-saturation relationship. Furthermore, this study suggests that interfacial area per volume is dependent upon the dominant flow mechanism (i.e. piston or finger) within the system, as well as, the connectedness of the wetting phase, thus providing valuable information that can not be obtained from the capillary pressure - saturation relationship alone.

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Locally conservative, stabilized finite element methods for mulitphase flow

Authors: C.E. Kees, M.W. Farthing, C.N. Dawson, C.T. Miller

It is well known that standard Galerkin finite element methods are inadequate for multiphase flow in porous media. Local oscillations can appear around sharp fronts without the use of mass-lumping, and velocity fields obtained from differentiation of pressure fields are discontinuous at element boundaries. For this reason, alternative approaches like mixed finite elements, discontinuous Galerkin methods, or control volume finite element approximations are usually preferred. Here, we consider conforming finite element discretizations based on a multiscale formulation along with recently developed, local postprocessing schemes. The resulting approach maintains the basic flexibility and appeal of traditional finite element methods, while controlling nonphysical oscillations and producing element-wise mass-conservative velocity fields. Accuracy and efficiency of the proposed schemes are evaluated through comparison with alternative, locally conservative methods for a series of steady-state and transient multiphase flow problems.

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Long-term injection of supercritical CO2 : Physical and chemical impact on the near-well zone

Authors: L. ANDRE, M. AZAROUAL

Geological CO2 sequestration offers a promising solution for reducing net emissions of greenhouse gases into the atmosphere. This technology has been successfully underway since 1996 in the Sleipner Field in the North Sea. In the framework of this concept, CO2 is injected into a saline aquifer in the supercritical state (P > 7.4 MPa and T > 31.1°C) in order to achieve a higher density and therefore occupy less volume underground. A pilot-project of geological CO2 storage in the deep Dogger aquifer in the Paris Basin (France) is under development. Before effective containment can be assured, investigations need to be carried out on reservoir behaviour when subjected to physical, chemical and mechanical perturbations induced by a massive and continuous CO2 injection. Numerical simulations using coupled hydrological and geochemical code are performed to study different scenarios of pure supercritical CO2 injection. Results of numerical simulations demonstrate that massive CO2 injection involves a major disequilibrium of the physical (temperature, gas saturation, pressure, capillary pressure…) and geochemical (dissolution of supercritical CO2 into the brine, pH variations, dissolution/precipitation reactions of the porous rock minerals) characteristics of the host aquifer. Firstly, supercritical CO2 dissolves into aqueous solution and it increases both water acidity and mineral dissolution potential, favouring augmented porosity. Nevertheless, after this phase, a prolonged CO2 injection period involves a desiccation phenomenon of the porous medium in the near-well zone. If in a first time, irreducible water, entrapped in micro-pores/micro-fissures, sustains the increase in CO2 pressure, when the pressure is sufficiently high and under a continuous dry (without water vapour) CO2 flux, advanced evaporation process allows the precipitation of salts and other secondary minerals. Porosity and possibly permeability of the host rock can be significantly impacted (decrease of rock porosity) influencing CO2 injectivity. Consequently, according to the position within the reservoir and gas saturation conditions, petrophysical properties of the host rock will evolve significantly during a long-term CO2 injection. Hence, the numerical simulations coupling flowing, thermal and geochemical processes seem to highlight that the near-well constitutes an underground hydrogeological system particularly impacted by supercritical CO2 injection. This zone appears as the most sensible zone where opposite chemical phenomenon (as dissolution/precipitation of some minerals) can have a dramatic impact. Moreover, according to injection temperature of supercritical CO2, major thermal variations, with an impact on hydraulic processes (as non-darcyan flow) and mechanical behaviour of the host rock (as micro fracturation), are expected. All these processes must be taken into account to evaluate the impact of CO2 injection on injectivity index and then conditioning a pilot and industrial operation success.

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Looking for 20th century climate change in Germany by means of stochastic time-series analysis of regional hydro-climatic data

Authors: Manfred Koch

For Germany, recent regional climate models have predicted significant seasonal changes of, mainly, temperatures and precipitation for the coming century that will require regional adjustments of the management of water resources, particularly, for agriculture. While the average citizen in Germany may have the perceived feeling that climate change, namely, a warming trend with summer extremes has affected the country several times during the last decade - also supported by meteorological measurements - it is still not clear whether such variations are just outliers in the observed hydro-meteorological time series with it's well-known stochastic nature, or whether they are just part of a long-term trend pattern that has already been ongoing over most of the 20th century. As part of a comprehensive study to understand the variability of stochastic hydro-climatic time series techniques, methods such as the Continuous Wavelet Transform (CWT), Detrended Fluctuation Analysis (DFA) and Singular Spectrum Analysis (SSA) have been applied to various hydro-meteorological data recorded over most of the 20th century throughout Germany and, namely, within several major river basins. As it is now commonly recognized that the observed variability of such climatic records can be characterized by a non-stationary stochastic process with a few periodic or nearly periodic components acting within time- scales that range from annual, over decadal, centennial to millennial and even longer time periods, the goal is to understand the exact nature of the stochastic process, namely, whether the various observed periodicities are an inherent property of the time series or if they are triggered by external events that act on more or less regular time-scales. Given the maximum record length of ~100 years in the present study, we are able to retrieve periodicities and the degree of persistence - as indicated by the calculation of the Hurst parameter with DFA - acting up to the decadal scale. Cross-correlations of the observed hydro-climatic time series with the North Atlantic Oscillation (NAO) - whose tele-connective effect on the European weather pattern on the inter-decadal scale has been surmised for some time, indicate a strong influence of the NAO on the long-term precipitation, though with somewhat different local effects throughout Germany. Extending the named analysis tools to discharge series in several river basins provides further evidence of such structural breaks in the time-series variability over Germany between the first and second half of the 20th century. While these results can somewhat be taken as indicators of some climate change that has been taking place in this country recently, the abnormal weather conditions experienced here in the last decade may then also be explained more as an inter-decadal intermittency phenomenon rather than as evidence for a long-term climatic trend.

Macroporosity of 2-D cross sections of soil columns via X-ray CT: multifractal statistics and long range correlations for assessing 3-D soil pore structure

Authors: M.A. Martín, F. San José Martínez, F.J. Caniego, M. Tuller, A. Guber, C. García-Gutiérrez, Y. Pachepsky

Soil pore structure controls important physical and biological processes in the soil-plant-microbial systems where microbial population dynamics, nutrient cycling, diffusion, mass flow and nutrient uptake by roots take place across many orders of magnitude in length scale. Over the last decades, fractal geometry has been proposed to deal with soil pore complexity and fractal techniques have been applied. Simple fractal models such as fractional Brownian motions, that have been proposed to capture the complex behavior of soil spatial variation, often cannot simulate the irregularity patterns displayed by spatial records of soil properties. It has been reported that these spatial records exhibit a behavior close to the so-called multifractal structures. Advanced visualization techniques such as X-ray computed tomography (CT) are required to assess and characterize the multifractal behavior of soil pore space. The objective of this work was to develop the multifractal description of soil porosity values (2-D sectional porosities) as a function of depth with data from binarized 2-D images that were obtained from X-ray CT scans of 12 water-saturated 20 cm-long soil columns with diameters of 7.5 cm. A reconstruction algorithm was applied to convert the X-ray CT data into a stack of 1480 grayscale digital images with a voxel resolution of 110 microns and a cross-sectional size of 690x690 pixels. The series corresponding to the percentage of void space of the sectional binarized images were recorded. These series of depth-dependent macroporosity values exhibited a well defined multifractal structure that was represented by the singularity and the Rényi spectra. We also parameterized the memory, or long range dependencies, in these series using the Hurst exponent and the multifractal model. The distinct behavior of each porosity series may be associated with pore connectivity and furthermore, correlated with hydraulic soil properties. The obtained multifractal spectra were consistent with multinomial multifractal measures where larger concentrations were less diverse but more common than the smaller ones. Therefore, models to assess pore space connectivity should incorporate a multifractal random structure compatible with this multinomial structure and the long range dependences that displayed these porosity series. Parameterization of the memory in depth dependencies of 2-D porosity series yields a useful representation of complex 3-D macropore geometry and topology.

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Mass and Heat Transport in Geothermal Systems

Authors: Karsten Pruess and Marcelo Lippmann, Earth Sciences Division, LBNL

Numerical simulation of fluid and heat flow in geothermal systems has seen continuous improvements since its beginnings in the 1970s. Complex three-dimensional models with thousands to tens of thousands of grid blocks are now routinely used by researchers and industry professionals. Although geothermal reservoir simulation has matured in some respects, major developments are continuing, often through cross-fertilization with other fields such as nuclear waste isolation, contaminant hydrology, and geologic storage of carbon. Active current developments include (1) methods for treating chemically and mechanically coupled processes, (2) techniques for automatic model calibration (history matching), (3) use of geophysical data for model building and testing, and (4) harnessing the power of PC clusters and multiple-processor hardware. This session aims to enhance the practical utility and reliability of geothermal reservoir simulation by strengthening the dialogue between practitioners and developers of numerical simulation tools.

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Massively Parallel Ultrascale Subsurface Simulation

Authors: Glenn E. Hammond, Peter C. Lichtner

Effectively harnessed, high-performance computation can have a significant impact on subsurface science by enabling higher fidelity simulations, increased chemical complexity and incorporation of multiscale effects through multiple interacting continua. The higher-fidelity simulations being executed on today's supercomputers have the potential of providing previously unattainable spatial resolution for large 3D simulations. Subsurface multiphase flow can now be simulated at finer scales that better adhere to hydrostratigraphy and with increasingly heterogeneous or stochastic parameter sets. Multicomponent biogeochemical transport can include an increased number of chemical components and reactions in multiple interacting continua. We present research being performed as part of the U.S. Department of Energy's SciDAC-2 (Scientific Discovery through Advanced Computing) program. As part of this program, we have been applying high-performance computation to better characterize and predict the movement of radionuclide contaminants at the Hanford 300 Area and the injection of sequestered carbon in the subsurface using the massively parallel code PFLOTRAN. PFLOTRAN is a multiscale, multiphase and multicomponent reactive flow and transport code founded upon PETSc data structures and solvers. It is the product of over 8 years of research and development in subsurface simulation and high-performance computation. We present simulation results from several of the largest subsurface flow and transport simulations executed to date on ultrascale computers (e.g. 10K+ processing units), involving the modeling of uranium geochemical transport at the Hanford 300 Area. Simulation of reactive transport at this site is complicated by stratified rock/soil layers with extremely high permeabilities, diurnal river fluctuations at the east boundary requiring refinement in temporal discretization, and highly nonlinear diffusion-limited mass transfer involving mineral and surface complexation reactions. We also discuss successes regarding our parallel implementation, roadblocks that we have encountered and overcome, and challenges yet to be surmounted.

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Mathematical and numerical models to predict migration distance of the CO2 plume in a geologic basin

Authors: Christopher W. MacMinn, Ruben Juanes

One of the major concerns in any geological CO2 sequestration project is the potential leakage of the CO2 into the atmosphere. Because the CO2 is less dense than brine, it tends to migrate upwards to the top of the geologic structure. The success of a sequestration project depends heavily on the mechanism of capillary trapping, by which the CO2 phase is disconnected into an immobile (trapped) fraction. In this paper, we develop mathematical models for the prediction of CO2 migration at the geologic basin scale. We present a one-dimensional sharp-interface model for the migration of CO2 in a porous layer. The model describes the gravity current of the buoyant CO2 during the injection period, as well as the wake of residual CO2 that forms during the migration of the CO2 plume after injection stops (this "secondary" migration is driven by buoyancy and regional groundwater flow). Until now, all sharp-interface models of gravity currents ignore the mobility contrast between the region fully saturated with brine, and the region with brine and residual CO2. We take that mobility difference into account, and develop a model that consists of two coupled nonlinear partial differential equations. Under certain realistic conditions, the governing equations reduce to a 2x2 system of hyperbolic conservation laws. We present the general analytical solution to the Riemann problem for this system (the Riemann problem is one in which the initial condition is a piecewise constant function with a single discontinuity). The front-tracking algorithm is then used to exploit the analytical solution for the simulation of the post-injection period, for which the initial condition (the geometry of the plume when injection ends) is far from a single discontinuity. The front-tracking algorithm also allows us to consider changes in the fluid properties (notably, the CO2 density and viscosity) as a function of depth along the migration path. Even though the models employed rely on a number of simplifying assumptions and only idealized injection scenarios are considered, they provide useful information regarding the expected footprint of geological CO2 sequestration projects at the basin scale.

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Mathematical modeling of microbial metabolic lag under exposure to heavy metals

Authors: Sema Sevinc Sengor, Petros Gikas, Timothy Ginn

Heavy metal toxicity has been observed in various aqueous systems, including wastewater streams, urban runoff and surface and groundwaters impacted by acid mine drainage. Most of the metals involved are toxic, mutagenic and/or carcinogenic to range of biotic species including microorganisms. The aim of this study is to develop a microbial growth kinetic model to simulate the transients in the metabolic activity of microbial cultures as a result of their exposure to toxic chemicals such as heavy metals. A metabolic lag factor appearing in the kinetics is developed as a convolution integral between a memory function and the local metals concentration to represent the activity of the microbial species as a fraction of their maximum activity (at metal free environment). The model is verified experimentally for a mixed microbial culture growing on acetate as sole carbon source, and in the presence of metal free, Ni, Co, Cr(III) or Cr(VI) contaminated environments. The data suggested that oxygen was limited in all cases due to insufficient transfer into the growth medium. This limitation was accounted through incorporating an interphase transfer flux for oxygen transport via diffusion within the Monod biodegradation kinetics. The effects due to the exposure to the heavy metals were captured in terms of increased lag and yield coefficient, despite the peculiar behavior of microbial growth due to oxygen limitation.

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Measures of Parameter Uncertainty in Geostatistical Estimation

Authors: Wolfgang Nowak

Within applied and theoretical studies of site exploration, measures of parameter uncertainty are required in order to assess the optimality of a suggested sampling scheme. These measures are particularly helpful when looking for an optimal experimental design that delivers the data required to reduce model uncertainty with minimum sampling effort. Along very different lines, research on data assimilation or geostatistical inversion techniques also requires measures of parameter uncertainty in order to assess the optimality of a certain conditioning scheme. Representing time series by a few temporal moments and asking about the associated loss of information is a common example. Regardless of the different context, the same kind of measures applies. For this purpose, a list of measures for parameter uncertainty is reviewed and discussed. Statistical significance, computational costs, and efficient ways for evaluation in specific situations receive a major focus. A first group of uncertainty measures is associated with so-called alphabetic criteria from the field of optimal design, including the A, D, E and C-criterion. They minimize the trace, determinant and maximum eigenvalue of parameter covariance matrices, and the prediction variance of dependent variables, respectively. A second group consists of rather intuitive measures commonly applied in the literature. For example, the averaged estimation variance (in Kriging-like procedures) or the correlation between a synthetic and an estimated field fall into this group. It is shown how these measures relate to the optimality alphabet in order to establish a solid theoretical background for them. Some new measures are also suggested in this study. Among them are the space-averaged conditional integral scale and a generalized set of measures relative to the prior uncertainty in conditioning schemes. Again, relations to existing measures from optimal design are shown, and the equivalence of the relative criteria to the concept of relative entropy is established. Relative entropy is a measure for added information through conditioning which is known from information theory and has been receiving elevated interest of the geostatistical and stochastic hydrogeological community recently. When applying these measures, mostly originating from the regression-like context, to geostatistical problems within the Bayesian framework, several issues of physical and statistical significance arise and are discussed. Also, computational feasibility is discussed and efficient ways to evaluate these measures are presented. As most general representative of linear or linearized spatial estimation within the Bayesian framework, this study is based on Cokriging generalized to uncertain mean and trends. Generalization to Kriging and quasi-linear schemes is straightforward. A major aspect to be kept in mind is that, in geostatistical applications, the number of parameters equals the number of discrete values for a random spatial parameter function. This number can easily reach the order of millions in 3D applications. The major conclusion is that the mean estimation variance and the averaged conditional integral scale are a powerful duo for characterizing conditional parameter uncertainty, and that they both have a direct correspondence in the well-understood optimality alphabet. This recommendation is in contrast to the fact that the D-criterion is the most commonly used in statistical literature. The D-criterion is rules out due to its computational complexity, unless the covariance structure among parameters allows swift computation of the matrix determinant. However, the relative D-measure introduced in this study offers an attractive alternative since it represents relative entropy and differs from the original D-criterion only by a constant.

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Micro-scale flow and transport studies in various porous geological media by lattice Boltzmann methods

Authors: Guoping Lu, Benjamin Gilbert, Liviu Tomutsa, Ming Zhang, Qinhong Hu, Qinjun Kang, Dongxiao Zhang

Flow and diffusion in geological porous media are fundamental processes governing solute and contaminant movement in the subsurface. These processes are traditionally studied by Darcy's law and the diffusive transport equation, respectively. However, it is not well understood in terms of the adequacy with which the continuum approach depicts fluid hydrodynamics and solute transport at the microscopic pore scale. The objective of this work is to understand the micro-scale flow and diffusion by fully describing micro-physical processes and implementing a kinetic model that is both suited to micropores and from which the familiar continuum relations emerge at the macroscale. We generated high-resolution x-ray CT tomograms for rock samples of various geological materials, including sandstones, limestone, tuff, and pore structure models of nanoparticle aggregates. These images represent pore structures for rocks (5-μm resolution) and nano-particle aggregates (5-nm resolution). We developed lattice Boltzmann models for simulating flow and diffusive transport processes in these pore systems. Preliminary results show that this approach can represent flow and diffusion in pores at a range of spatial scales. Studies of diffusion within nanoscale pores show that pore morphology can attenuate solute transport by several orders of magnitude compared to bulk water.

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Microbial metabolism in reactive transport models of porous media: Approaches, Potential and Limitations

Authors: Christof Meile, Eric King, Kagan Tuncay, Peter Ortoleva

Microbes control the breakdown of organic matter in low temperature subsurface environments, drive elemental cycling, and determine the fate of many contaminants. They affect the physico-chemical nature of their surroundings either directly or indirectly, and in aggregate, microbial populations can alter the bulk redox conditions such that there arises a strong feedback between the environmental conditions and microbial community composition. Quantifying the complex and dynamic interactions between numerous concurrent biogeochemical processes necessitate the use of mathematical models that include representations of transport, chemical reactions and microbial activity. Historically, reactive transport models have ignored the microbial dynamics all together or included them in rather simplistic fashion (e.g., Thullner et al. 2007. Geomicrobiology Journal 24: 139-155). Despite their success in reproducing observed geochemical zonation, it is evident that such representations of microbial metabolism employed neither reflect the natural complexity nor diversity. To truly understand the effects of microbes and feedbacks with the environment, one needs insight into the community composition, their metabolic capability, and in situ activities; and for predictions, the response to outside forcing is required. The extensive knowledge gained at the molecular and genetic level with onset of the biological revolution provides the opportunity to develop explicit models of cellular metabolism. Paired with the in situ characterization of microbial ecology and specific laboratory experiments, this ultimately allows implementation of the subsurface microbial activity in a more realistic fashion. Here we present efforts toward an integration of the newly available biological data into reactive transport models. We are tackling cell-internal processes by comparing steady-state flux balance approaches and dynamic cell models, and we then study microbial dynamics in porous media settings. We compare cell models, differing in i) the extent of the metabolic network considered and ii) the level of detail individual processes are described. Specifically, we contrast different flux balance models of Geobacter sulfurreducences, an abundant and metabolically versatile delta-proteobacter whose genome has been sequenced (Methe et al. 2003. Science 302:1967-1969), with a kinetic cell model and assess the respective advantages and potential shortcomings. To highlight their similarities and differences, growth efficiencies are computed and compared to observations. While only the kinetic model includes explicit expressions that relate substrate uptake to concentrations in the outside world, for a given substrate uptake flux, both the flux balance models and kinetic cell model provide similar results and match the experimental data quite closely. At low acetate uptake fluxes, acetate mainly fuels the TCA cycle, while at higher uptake rate, the relative contribution to growth increases. To identify key components determining model behavior, a sensitivity analysis is performed by quantifying the effect of parameter perturbations on the deviation of process rates from steady-state conditions. These simulations support that energetic status and intracellular substrate concentrations affect growth rates. We then explore the role of pore scale variability by combining cell-model derived growth efficiencies with explicit representations of the granular structure of porous media. Under parameterization representative of environmental conditions, our simulations indicate that advective fronts or limited pore connectivity is required to establish significant heterogeneity at the grain scale. Finally, we discuss the impact of model simplifications, and comprehensiveness of the reaction network considered at the scale of a contaminant plume.

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Mixed finite element and multi point flux approximation of variably saturated subsurface flow with simultaneous multicomponent reactive transport

Modeling alternative heat pulse probe designs for improved estimations of thermal and hydrological properties

Authors: Tamir Kamai, Atac Tuli, Gerard J. Kluitenberg, Jan W. Hopmans

Soil thermal and hydrological properties have large impact on biophysical, biochemical and microbiological processes, and are also important for quantifying climate change effects on these processes. Most of these processes are temperature dependent and require knowledge of soil thermal properties for accurate predictions of soil temperature and its influence on seed emergence and crop growth, soil water retention and unsaturated hydraulic conductivity, and soil water vapor flow in coupled water and heat transport. The heat pulse method, with the heat pulse probe (HPP), has been successfully used for in-situ estimations of soil thermal and hydrological properties, i.e., thermal conductivity, volumetric heat capacity, thermal diffusivity, water content and water flux density. However, measurements of water flux density are limited to 5 cm per day, whereas vadose zone fluxes are generally lower than 1 cm per day. Furthermore, the current HPP design has low durability for field applications. In the study presented herein, both of these HPP limitations are addressed by using a combination of analytical and numerical solutions, coupling heat and water flows. Finally, these solutions are validated by inverse modeling with measured data. Sensitivity analysis was conducted with these models, and included varied heater needle diameter, thermistor-heater needle distance and heating pulse pattern. Results from this analysis suggest that larger heater needle diameters combined with a different heat-pulse pattern are required to make lower unsaturated water flux measurements possible. By constructing a large-heater HPP, water flux of 1 cm per day was successfully measured and inversely estimated. For enhancing probe durability, a short-needle probe was evaluated. The new short-needle geometries preclude use of analytical solutions, in which numerical solutions are required. We show that data from a short-needle HPP can be predicted with these numerical solutions, making this probe applicable and robust.

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Modeling and inversion of self-potential signals associated with flooding events at the Thur River, Switzerland

Authors: Niklas Linde, Oliver Genoni, Joseph Doetsch, Stefan Finsterle

Several field-based studies are currently underway to understand naturally occurring electrical potential (self-potential) variations associated with hyporheic processes. We monitor self-potentials in the vicinity of the Thur River, which is located in northern Switzerland, to (1) examine the validity of a newly developed formulation of self-potentials associated with multi-phase flow processes, and (2) investigate to what extent the self-potential method can provide information about flow processes in the hyporheic zone. We incorporate a two-dimensional integral finite-difference formulation of the multi-phase self-potential problem in the hydrological inverse code iTOUGH2. For accurate modeling, we implement a petrophysical model to calculate the time-varying electrical conductivity of the sediments as a function of state variables such as water saturation and salinity, as well as space-varying surface conductivity. Time-lapse self-potential data can be used to invert for flow parameters since the source currents and the resulting self-potentials are strongly affected by hydrological state variables, such as the pore water velocity. A synthetic example shows that the effective hydraulic conductivity can be retrieved from self-potential data if the petrophysical properties of the porous media and the temporal variation of the river stage are known. Laboratory studies of sediment samples indicate that the saturated voltage coupling coefficient of the gravel deposits at a pore water conductivity of 0.34 mS/m is -20 mV/m. A simulation of a hypothetical flooding event predicts that self-potential anomalies of up to 10 mV can be expected at the Thur River. Self-potential data are monitored with a self-potential monitoring network based on a data logger and 16 non-polarizing Pb/PbCl2 Petiau electrodes. We present data collected over several weeks (1) on a gravel bar (250 × 50 m2) in a restored section of the Thur River, (2) on a flood plain located in the vicinity of an unrestored section of the Thur River, and (3) in four neighboring boreholes. In the surroundings, we collected regional-scale self-potential information during stable weather conditions. We first qualitatively reproduce the observed self-potential signals using the modified iTOUGH2 code. When a similar signature for both the observed and simulated signals is established, we invert the observed SP data for an effective hydraulic conductivity of the gravel deposits. This model allows us to estimate the residence time in the gravel bar and to relate the self-potential signals observed on the flood-plain with variations of the water table associated with rapid fluctuations of the river stage. We conclude that self-potential data provide an independent and valuable data source for constraining flow models of the hyporheic zone. We stress that quantitative integration of self-potential data in a formal hydrogeophysical inversion should only be attempted when reliable petrophysical and electrical conductivity models are available.

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Modeling evaporation from a non-vegetated lysimeter experiment

Authors: Philip H Stauffer

We present results from a numerical study of near surface evaporation in the absence of vegetation. Two numerical approaches are used to fit mass balance data from a weighing lysimeter in the Mojave Desert. Both approaches attempt to match the time history of the mass of the lysimeter using the daily precipitation record as input. The first approach is physics based, relying on gradients in water vapor pressure to drive evaporative flux to the atmosphere from the top of the soil. We assume fixed relative humidity in the atmosphere and assume that soil properties are known. To fit the model to the lysimeter data, we adjust only the effective porous medium diffusion coefficient in the near surface. This model gives very good agreement to the character of more than 10 years of data; however, the two curves diverge at three rainfall events. Removal of the excess moisture in the simulated lysimeter during these three events causes the model/data correlation to improve dramatically, suggesting that some vegetation may have been removing moisture over brief periods during the experiment. The second approach presented uses a purely empirical technique. We extract the derivative of the weight of the lysimeter through time as a function of the saturation in the top of the numerical grid while the simulation is forced with the measured time history from the site. The resulting curve is then simplified to a function that is used to drive a simulation of the site. Results from this method do not follow the shape of the data curve as closely; however the long term results tracks the data very well while requiring no removal of precipitation. Both approaches proved highly dependent on grid spacing in the near surface. Interestingly, both were well fit with a grid spacing of 20 cm across the land-air interface.

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Modeling Flow and Nitrate Transport in a Deep Alluvial Vadose Zone: different Approaches for Characterizing Subsurface Heterogeneity

Authors: Farag Botros, Thomas Harter

We developed three different representations of a 16 m thick, alluvial unsaturated zone. The first is a homogeneous lithofacies representation which explicitly identifies major textural facies within the unsaturated zone. The second is a heterogeneous lithofacies model which includes heterogeneity within each facies using scaling factors technique. The third is also a heterogeneous model where the heterogeneity in each lithofacies is characterized by using different random fields of each van Genuchten parameters. Methodology to generate random fields of scaling factors and van Genuchten parameters is explained where autocorrelation and cross-correlation between parameters is honored based on an extensive measurement and laboratory analysis in an irrigated orchard in semi-arid Fresno County, California. We also compared the effect of these three heterogeneity representation on water flow and nitrate transport. Transient, two and three-dimensional water flow and nitrate transport processes are simulated over seven years beneath two fertilizer treatments. Estimated nitrate levels in the vadose zone and nitrate leaching to groundwater are significantly different between the fertilizer treatments, yet are nearly identical between the three models. In all cases, the deep vadose zone nitrate mass is at least four times larger than the measured nitrate mass at the site. The high discrepancies between the measured and model estimated nitrate at the site underscore the need for a rigorous examination of alternative modeling strategies to simulating deep vadose zone flow and transport processes.

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Modeling Flow and Reactive Solute Transport in Multi-scale Fractured Rock

Authors: Zhenxue Dai, Andrew Wolfsberg, Zhiming Lu, George Zyvoloski

In order to test concepts of parameter scaling from bench-scale fractured-rock column experiments to kilometer-scale fracture network characterization, we have developed a multi-scale transition probability model to simulate the geometry of fracture network systems and at the same time to upscale the fracture apertures and fracture block proportions. Flow and reactive solute transport in the upscaled fracture network are simulated with a novel generalized dual-porosity model (GDPM) implemented in Los Alamos National Laboratory\'s FEHM groundwater flow and transport simulator. The GDPM formulation provides high numerical resolution in secondary matrix nodes near the primary fracture nodes, which enables highly efficient and accurate simulations of diffusive concentration fronts moving between fractures and matrix material. In this presentation, we first describe the geometry simulation of a two-family orthogonal fracture network with an indicator cokriging method based on the multi-scale transition probability model. Then we evaluate the scaling affect for flow and transport in the fracture network system that account for heterogeneity in diffusion coefficients, apertures, and radionuclide sorption parameters. The developed methodologies will be applied for identifying the preference paths for reactive solute transport in fractured rock.

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Modeling Flow and Sediment Transport of the Chesapeake Bay

Authors: Nitin Bedi, Jin-Ping (Jack) Gwo

The Chesapeake Bay is the largest of the 130 estuaries in the United States. With over 200 miles in length and draining a 64,000 square mile watershed, it is one of the most productive and valuable natural treasures of the nation. However, the high land-to-water ratio within the watershed (64,000 to 4,500 square miles), which encompasses geographically the densely populated District of Columbia and Baltimore metropolitan areas, greatly influences the health of the Bay. Increasing population and the pollution in the land, water and air in the watershed has negatively impacted the resources in the Bay and significantly lowered the quality of life in its waters. Non-point source pollutants such as sediment, nutrients, and certain heavy metals wash into the Bay from the land surface and rivers. Sediments make the water turbid thereby preventing the sunlight to reach the submerged aquatic vegetation at the bottom of the Bay, which in turn impact the habitats of other aquatic lives and the important aquacultures of the region. They also carry with it nutrients and toxic chemicals which contaminate the water. Though much work is done in predicting nutrient pollution, much remains to be studied about sediment sources and transport. This study aims at calculating the flow patterns and the transport of sediment in the Bay. The goal is to develop a mechanistic-based, first-principle model that incorporates field and laboratory measurements that may eventually reduce model prediction uncertainty in the event that the model is to be used in predictive mode and be incorporated into a mechanistic-based watershed model that takes into account, among others, urbanization, climate change, point and non-point source pollution (e.g., agrichemical and pharmaceutical pollutants), and the interaction of surface water and groundwater that remains to be a critical water resource of the region. Finite element and the method of characteristics are used to solve the flow and transport equations for the Bay. The Bay is a shallow water body and is approximated by a two dimensional numerical model. A 2-D finite element mesh of the Bay is developed on the basis of publicly available digital bathymetry maps. Measured discharges from the major rivers of the Bay and tidal input from the ocean are applied as boundary conditions. The flow simulation outcomes are similar to those obtained from other simulation results, e.g., the NOAA C3PO model, at the macro scale. Our 2-D model, without taking into account the salinity and wind stress effects in the Bay, predicted more local circulation patterns. These findings point to the needs of incorporating these effects when detailed calibration of the model is feasible. For the purpose of this study, we are more interested in the macro scale flow patterns that may impact the transport of sediments. Thus, once a steady state flow pattern is reached in the 2-D model, the flow field is used for the subsequent sediment transport simulations. For sediment transport calculations it is assumed that all sediments are uniformly distributed in the bed of the Bay initially. Only subsequent sediment inputs to the Bay from the major rivers, not the lands, were considered in the model. The transport simulation produced physically reasonable results and suggested that hydrodynamics may impact the redistribution of bed and river sediments. However, the deposition and erosion equations and their associated parameters in the model may need to be further calibrated by using large-scale field data, which is mostly absent at this moment, before the sediment transport model is fully amenable to studying the mechanisms of natural and anthropogenic impacts to the bay and estuarine system.

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Modeling Groundwater – Surface Water Exchange on different scales: the Lowland River Spree example (Germany)

Authors: Gunnar Nützmann, Dimitri Peyrard, Michael Decker, Jörg Lewandowski

The hydrology of the exchange processes between surface water and groundwater as well as biogeochemical turnover processes affect the quality of both water bodies. Therefore, understanding of local flow and mass transport mechanisms is important for water management. Especially in lowland basins relatively low flow velocities in rivers and hydraulically highly permeable aquifer sediments lead to an intensive exchange between surface and subsurface water, which is mainly controlled by transient water levels. To find out more about the involved processes and to understand the feedbacks of these coupled processes across the hydrologic cycle we conduct investigations at a study site surrounded by the current river bed and an old branch of the lowland River Spree, a 6th order river, near Freienbrink, north-eastern Germany. Water levels and temperature in the River Spree, in its old branch and in 12 groundwater wells of a 300 m long transect are collected automatically with data loggers in order to model groundwater recharge and water exchange between surface water and groundwater. Normally, a hydraulic gradient in the aquifer causes groundwater flow into the stream. However, water level fluctuations of the stream spread out surprisingly quickly in the near-surface aquifer of the floodplain. As a result, an inverse hydraulic gradient and infiltration of surface water into the aquifer and temporary bank storage take place. We investigate with the help of two different modeling approaches a) the spatial and temporal groundwater and river flow in a meso-scale, and b) based on this results on a local scale, how deep into the aquifer surface water infiltrates, how fast this infiltration takes place and whether there are stable mixing zones in the aquifer. The meso-scale model consists of fully coupled horizontal 2D Saint Venant equation for river flow and a 2D Dupuit equation for aquifer flow. The dynamic coupling between river and aquifer is provided by continuity of fluxes and water level elevation between the two domains. For simulating the local flow within the second modelling approach a transient 3-D groundwater model was developed using MODFLOW and the River Package describing the surface – subsurface water exchange. The meso-scale model accurately reproduces the strong hydraulic connections between the Spree River and the aquifer that are confirmed by the simultaneous variation of the water level in the river and in piezometers located near the river bank at the study site. The simulations also confirmed that the model is able to reproduce spatial and temporal changing groundwater flow dynamics during seasonal flood events. The 3-D local model was applied to the study area simulating an annual hydrological cycle. The calculated water levels fit the observed ones very well and varying areas of interactions between the River Spree and the aquifer has been detected. Given these results, both hydraulic models can be coupled with solute-transport models, based on advection-dispersion equations, to investigate the dynamics of conservative and reactive components in this coupled groundwater-surface water system.

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Modeling Hydraulic Responses to Meteorological Forcing:From Canopy to Aquifer

Authors: Lehua Pan, Jiming Jin, Norman Miller, Yu-Shu Wu, Gudmundur Bodvarsson

An understanding of the hydrologic interactions among atmosphere, land surface, and subsurface is one of the keys to understanding the water cycling system that supports terrestrial ecosystems. Properly modeling such interactions is difficult because of the inherently coupled processes and complex feedback structures among the subsystems. In this paper, we present a model that simulates the land-surface and subsurface hydrologic response to meteorological forcing. This model combines a state-of-the-art land-surface model, the NCAR Community Land Model version 3 (CLM3), with a variably saturated groundwater model, TOUGH2, through an internal interface that includes flux and state variables shared by the two submodels. Specifically, TOUGH2 uses infiltration, evaporation, and root-uptake rates calculated by CLM3 as source/sink terms; while CLM3 uses saturation and capillary pressure profiles calculated by TOUGH2 as state variables. This new model, CLMT2, preserves the best aspects of both submodels, specifically, the state-of-the-art modeling capability of surface energy and hydrologic processes from CLM3 along with the more realistic physical-process-based modeling capability of subsurface hydrologic processes from TOUGH2. The preliminary simulation results show that the coupled model greatly improves predictions of the water table, evapotranspiration, surface temperature, and moisture in the top 20 cm of soil at a real watershed as evaluated from 18 years of observed data. The new model is also ready to be coupled with an atmospheric simulation model to create one of the first models capable of simulating hydraulic processes from the top of the atmosphere to the deep-subsurface.

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Modeling iron (hydr)oxide reductive dissolution and metal transport in mining-impacted riverine and lacustrine sediments

Authors: Nicolas Spycher, Arash Massoudieh, Sevinc Sengor, Tim Ginn, Brent Peyton, Rajesh Sani, James Moberly

It is estimated that ore mining activities have contributed to the degradation of 4,000 to 10,000 miles of streams in the Western U.S, resulting in the loss of aquatic life, and restrictions of stream use for recreation, public drinking water and industrial water supplies. The Lake Coeur d'Alene River and Lake Coeur d'Alene itself, located in northern Idaho, are prime examples of such impacted areas. The sediments of both the river and lake at the delta have been impacted by decades of contaminated runoff, mainly from the Bunker Hill mining area. These sediments show high bulk concentrations of Fe (~15% by weight as Fe2O3) and Mn (2% by weight as Mn2O3) together with elevated concentrations of Zn, Pb, Cu and other toxic metals. Nanoparticulate Fe and Mn (hydr)oxides generated by the mixing of acid mine drainage and surface waters could significantly contribute to the transport of metals downstream from mining areas (as sorbed species), along with the transport of detrital primary sulfide minerals. Historically, in the case of Lake Coeur d'Alene, there has been a controversy over whether metals in the lake sediments are primarily associated with iron oxides or sulfidic phases. Relatively recently, spectroscopic measurements by others have shown abundant ferrihydrite and high Fe-to-S ratios in the sediments, providing support that metal transport to the lake could occur primarily as sorbed species onto Fe(III) (hydr)oxides. On the basis of these investigations, we recently developed a PHREEQC-based diffusive-reactive transport model to evaluate the mobilization of heavy metals sorbed onto ferrihydrite by means of microbial reductive dissolution, and the competing effects of metal precipitation as biogenic sulfide minerals. The model showed that these processes could dominate the biogeochemical behavior of heavy metals in the sediments. Here, the modeling effort is extended to assess the dissolution of primary (detrital) sulfide phases as another potential source of dissolved metals, and the role of detrital sulfide minerals as potential electron donors for the abiotic and/or biotic reductive dissolution of ferrihydrite. Simulations consider redox disequilibrium and sorption is treated by a full surface complexation model. The model incorporates a multicomponent biotic reaction network with multiple terminal-electron acceptors and nonlinear kinetics to capture electron-acceptor limitations on degradation rates as well as inhibition by presence of alternative electron-acceptors.

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Modeling of Chemical, Thermal, Hydrological, and Mechanical Effects on Geomaterial Performance

Authors: Jan van der Lee, Ecole des Mines de Paris - Centre de Géosciences and Carl I. Steefel, Lawrence Berkeley National Laboratory

The long-term performance of engineered and natural geomaterials is of concern to earth and environmental scientists and engineers in a number of applications and settings today. Some notable examples include the performance of nuclear waste repositories that rely on both natural and engineered barriers to retard radionuclide transport, the behavior of natural (e.g., shale) and engineered (e.g., cement) seals for deep aquifers proposed for CO2 sequestration, and the leaching of solid waste forms such as those used in road or building construction. The performance of these geomaterials can be affected over the long term by chemical, thermal, hydrogical, and mechanical processes acting individually or acting together in a coupled fashion.

To address these concerns, there is increasing interest in developing quantitative, scientifically defensible models for the coupled processes that affect geomaterials, particularly where their performance must be assured for long, often geological periods of time. For this session, we invite state-of-the-art contributions in mechanistic modeling of geomaterial performance in any application of broad interest to earth and environmental sciences. Contributions might range from those focusing on new numerical approaches to modeling highly coupled thermal-hydrologic-mechanical-chemical (THMC) systems, to those investigating the behavior of geomaterials in the real-world setting of a proposed nuclear waste repository or deep aquifer.

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Modeling of Connectivity in 3D Continuum Systems using Percolation Approach

Authors: Alireza Hajizadeh, Mohsen Masihi

Uncertainty in reservoir performance arising from lack of precise knowledge of the subsurface is a key factor in the risk assessment of field development. The conventional approach to estimate this is to build detailed geological models which are then upscaled to a coarser grid where flow simulations are run. The whole process is repeated for other possible stochastic realizations of the reservoir and/or further repeated for alternative development scenarios. All these are generally far too time consuming to be carried out practically. An alternative approach is to use a much simpler modeling scheme with the aim of predicting flow behavior and its associated uncertainty very rapidly without generating realizations of the system. In this study we use a simple object based technique based on the percolation theory by first simplifying the reservoir permeability map to either permeable (e.g. sand) or impermeable (e.g. shale). We further assume that the controlling parameter in flow is the bodies connectivity. With these we use percolation concepts in simple algebraic relations in 3D models to estimate the connectivity of both isotropic and anisotropic systems extremely rapidly.

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Modeling of Subsurface Biogeochemical Processes

Author: Carl I. Steefel, Lawrence Berkeley National Laboratory and Pierre Regnier, Utrecht University

Biogeochemical processes have a major impact on water quality and the management of water resources, through the important role they play in a number of subsurface environments—ranging from soils and shallow sediments, to drinking water aquifers, to deep gas or oil reservoirs. Biogeochemical processes are also the key element in the natural attenuation of contaminants, and are now being manipulated in various bioremediation schemes intended to accelerate contaminant cleanup. However, our understanding of the functioning of microbially mediated biogeochemical processes in the subsurface is still inadequate. While this results in part from the need for additional fundamental research, it also reflects the need for a new generation of fully coupled biogeochemical transport models that can capture quantitatively the complex interactions between the subsurface environment and the resident biota, across a wide range of scales.

This session will focus on innovative approaches to modeling subsurface biogeochemical processes. Topics to be considered include interactions among subsurface transport, biogeochemistry, and microbial processes across multiple scales, the representation of microbial processes and the biosphere in reactive transport models, bioenergetic constraints on microbially mediated processes, element and nutrient cycling as a result of biogeochemical processes in soils and shallow sediments, and the incorporation of isotope systematics into biogeochemical models to improve the constraints on reaction networks and rates.

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Modeling rhizoshere soil mechanics and hydraulics - an overview

Authors: Markus Berli, Teamrat A. Ghezzehei, Manoj Menon, Scott W. Tyler, Michael H. Young, Anthony R. Dexter

The rhizosphere encompasses the volume of soil surrounding living plant roots and is strongly modified by plant activities. Root growth, uptake of water and nutrients, secretion of mucilages alter the physical, chemical, and biological properties in this region. Of these, the impacts on physical properties have received little attention. In this work we show some potential interactions between plant roots and soil mechanical and physical properties using numerical modeling the hydrological and mechanical changes that accompany growth of a single plant root. Our simulations show how root activities alter the mechanical and physical properties (such as density, water retention characteristics) and how these alterations in turn impact water delivery to the plant roots.

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Modeling root water uptake based on the distribution of water potential in soil and root

Authors: Javaux

Root water extraction from soil is controlled by the distribution of local water potential gradients between soil and root segments. However taking this local effect in consideration is challenging given the lack of real data on root architecture, on the distribution of the water potential at the root-soil interface, or on the local hydraulic properties of soil and root. In order to numerically investigate the water uptake processes at the plant scale, we built a 3-D model, called R-SWMS, which combines water flow in conducting vessels of a plant and within the soil matrix. The distribution of the soil-root water fluxes is calculated based on the water potential gradient and the local hydraulic properties of the root and the soil. The effect of the soil type and root architecture on the extraction pattern and the root collar fluxes is investigated with a sensitivity analysis. Depending on the plant transpiration and the soil water status, the highest resistance against flow occurs in the soil or in the plant. It is shown that it is impossible to derive simple, straightforward conclusions on a sink term distribution or root uptake processes based on 1-D averaged datasets. The problem of the soil and root discretization is also addressed. The issue to be solved is how to estimate the local soil-root water fluxes when multiple roots are located in one voxel. We study this problem by comparing different solutions for simplifying the geometry and the boundary conditions of the water flow problem below the soil voxel scale. Subsequently, we compare this 3-D model with alternative modeling approaches for root water uptake.

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Modeling the Hydrology of California's Sierra Nevada for Sub-Watershed Scale Adaptation to Climate Change

Authors: Chuck Young, David Purkey, Marisa I. Escobar, Martha Fernandes, Brian Joyce, Michael Kiparsky, David Yates

In collaboration with the Center for Watershed Sciences at UC Davis and funded by the Resources Legacy Fund Foundation, the Stockholm Environment Institute has developed hydrology models for the western slope of the Sierra Nevada from the Feather to Kern River watersheds. The models were developed to provide hydrologic simulations at a finer spatial scale than has been previously attempted in the Sierra for use in assessing the local impacts of climate change and operations management on hydropower projects. The models calculate many aspects of the hydrologic cycle including snow accumulation, snow melt, surface runoff, infiltration, interflow, and base flow. Weekly predictions of unimpaired stream flows were made at 261 locations throughout the 15 watersheds for the time period 1982-2001. Model input included precipitation, temperature, and wind data which allowed for analysis of climate change scenarios through the alteration of the input weather data. Calibration was conducted using stream and snow observations internal to the watersheds for the time period 1982 – 2001. In a departure from previous efforts at Sierra wide hydrological modeling, a uniform set of calibration parameters was applied to the entire study area and model validation was conducted by comparing flow predictions at USGS gauge sites internal to the watersheds and by comparing flow predictions at the bottom of the watersheds to calculated DWR full natural flow volumes. Runs of the model for climate change scenarios with fixed increases of 2, 4, and 6 degrees Celsius for the whole modeling domain were used to perform first and second order analyses. First order analyses of calibrated outputs indicated reduction in snow melt volume that is most dramatic at the 1750-2750 m elevation range. In addition, the runoff center of mass shifted to earlier dates and was non-uniformly distributed throughout the Sierra Nevada. Examples of second order analyses of non-calibrated outputs such as evapotranspiration and soil moisture indicated increases in potential evapotranspiration and reductions in relative soil moisture for scenarios with higher temperatures which are more pronounced at higher elevations. Because the hydrologic model presented here is dynamically linked to a highly developed water resources planning tool, future research opportunities derived from the analytical platform include analysis of climate change impacts on water allocation and watershed ecosystems to examine potential adaptation strategies.

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Modeling the hysteretic behaviour of the moisture retention curves of peat soils in the Zennare Basin, Italy

Authors: Francesca Zanello, Mario Putti, Pietro Teatini

Peatlands respond to natural hydrologic cycles of precipitation and evapotranspiration with reversible deformations mainly because of the variation of water content in the unsaturated zone. The modeling of water infiltration in these type of soils must include an accurate description of the characteristic capillary retention curves. Recent measurements obtained from a field experiment in a peaty soil in the Zennare Basin (located south of the Venice Lagoon in Italy) show a strong hysteretic behaviour of the water content-suction relationship even at relatively high water content values. The characterization of this functional relationship is of primary importance for accurate hydrological simulations. An in depth analysis of the field data measured over a period of more than two years shows a clear influence of temperature on moisture retention relationship. A simple Fourier analysis of these data confirms that the principal modes of the recorded moisture and suction time series coincide with those of thermal fluctuations. The algorithmic approach proposed by Haverkamp et al. (2002) for sandy soils has been implemented in a Richards\' equation simulation code that incorporates also swelling/ shrinking dynamics of peat soils. The numerical model discretizes Richards\' equation by means of linear finite elements combined with Euler time stepping. Mass lumping is also used to increase the stability of the overall approximation. The resulting nonlinear system of equation is solved using the Picard technique, so that linearization is achieved by evaluating of the nonlinear terms at the previous iteration level. This approach allows an easy localization of the reversal points within the hysteretic curve family that can be updated within each Picard iteration. To improve the numerical performance, a specific algorithm has been implemented to smooth possible non physical hysteretic loops that are created by small numerical oscillations and corresponding capillary pressure variations. The model has been then applied to a peat column representative of the actual situation found in the Zennare Basin.The simulated capillary pressure and moisture content behaviour does not show the expected strong contribution of the hysteretic effect to the water dynamics in the vadose zone. The main reason for this negative result may be related to the fact that the geometric scaling, the basis of Haverkamp\'s approach, cannot be extended to peats and probably apply only to sandy soils. We study how this model can be modified to extend its applicability also to organic soils. Processes that will be taken into in the new modeling efforts must include temperature effects and soil porous space variations due to the nonlinear swelling/shrinking phenomena. To more accurately study the interactions between these processes, we are starting to develop a Ising-type microscopic model with which all these different dynamics can be potentially described. This model builds upon similar work carried out in the field of filtration theory and will be used to develop and verify new algorithmic approaches for the implementation of this type of hysteretical effects on Richards\' equation.

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Modeling the impact of gasoline hydrogenates (particularly MTBE and Ethanol) on the persistence of BTEX compounds in a gasoline- contaminated ground water site in Iran, using RT3D code.

Authors: Mahsa , Behzad

To evaluate and comprise the effect of common fuel additives,MTBE and Ethanol, on BTEX fate and transport and natural attenuation in a fuel- contaminated groundwater site located in central Iran, we have used RT3D code(Clement et al, 1998), and a newly developed module for this model (Gomez et al, 2007).This module includes commonly considered fate and transport processes such as advection, dispersion, adsorption, aerobic and anaerobic biodegradation, and depletion of molecular oxygen during biodegradation. Also it involves terms for simulating substrate interactions previously not take into account. Terms such as: (1) decrease in the specific BTEX utilization rate due to ethanol preferential access to electron acceptors particularly oxygen, (2) repression of inducible enzymes that degrade the target pollutant (e.g., benzene) by the presence of preferred carbon source (e.g., ethanol), and (3) growth of different microbial populations in response to changes in oxygen and substrate availability. In this study we examine 3 conceptual model firstly, to evaluate the transport and natural attenuation of BTEX compounds in absence of any oxygenate additive assuming Kinetic-limited degradation of BTEX using multiple electron acceptors which is one of the predefined modules exist in RT3D code, secondly to estimate the impact of ethanol on the persistence of BTEX compounds in gasoline contaminated groundwater, and third, to compare the length of BTEX plume in second scenario with the length of BTEX plume in a site contaminated by MTBE-blended gasoline. The 3 conceptual models are: 1. A spill/leak of gasoline (no additive compounds) as a base case. 2. A spill/leak of gasohol (10 percent v/v known as E10) into a pristine aquifer. 3. A spill/leak of MTBE-blended gasoline (15 percent v/v) into a pristine aquifer. The physical hydrogeologic parameters used in simulations, and Biodegradation rate parameters were derived from former field-studies and literature values. A shallow, water-table sand aquifer with minimum geological complexity are considered. The simulations were run for 10 years, and the BTEX source concentrations was simulated as a constant concentration of 13.7 mg/lit. An ethanol concentration of 1000mg/lit and a benzene concentration of 10mg/lit was assumed to exist at the source zone. Plume length was defined as the distance from the source to the 5µg/l contour. The simulations results show that the presence of ethanol in E10 can cause benzene plume elongation by 20-60% in compare to the base scenario, depending on the condition of source point. This is in good agreement with previous studies of benzene/ethanol plume length. By substituting some parameters values in the source code of module, and running the third conceptual model, results demonstrate that MTBE plume were longer and wider than benzene plume. Given the similarities between the dimensions of benzene and MTBE plumes, and the similar biodegradation rate estimates obtained for benzene and MTBE it is reasonable that no significant changes would be observed in the elongation of MTBE-blended gasoline in compare to the base scenario. Finally, a sensitivity analysis of the system was performed to assess the most influential variables involved in the system. For the base scenario (natural attenuation BTEX plume with no additives), The results of a sensitivity analysis show that the saturated aquifer thickness, hydraulic conductivity, and reaction rate constants are the most critical parameters controlling the natural attenuation of ETEX at this site. For second and third scenarios Variables such as porosity, hydraulic conductivity, hydraulic, also source zone concentration and biofilm density are important values. The substrates aerobic and anaerobic kinetics follow in importance. However, in general system is not largely sensitive to changes in a single variable.

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Modeling the Interactions among Microbial Communities under Environmental Conditions through High Density Phylogenetic Microarrays.

Authors: Curtis Luce, Joe Song, Todd DeSantis, Eoin Brodie

Curtis Luce (New Mexico State University, Las Cruces, NM 88003), Joe Song (New Mexico State University, Las Cruces, NM 88003), Todd DeSantis (Lawrence Berkeley National Laboratory, Berkeley, CA 94720). Eoin Brodie (Lawrence Berkeley National Laboratory, Berkeley, CA 94720). The K-th order logical network modeling software determines significant interactions among microbes in a microbial community and environmental factors influencing microbial distributions. Using inference of the K-th order the temporal information in 16S rRNA microarray (PhyloChip) data-sets provides a basis to examine microbe-microbe and microbe-environment interactions using the logical network model. In a logical network, a logical function, associated with each microbial species as a node, describes its behavior dictated by some other influential microbes or environmental factors. The optimal logics at each microbe node in the network will be searched so that they best explain the observed data. Determination of an optimal logic will involve parent node selection and truth-table generation. The maximum number of parents is set to a given number. If the current node shows consistent behavior during transition from one state to another given the parent nodes, then the parent nodes will be kept. The actual goodness of the transition will be calculated using the chi-square test. The modeling will be used to inspect sewage-impacted urban water quality and the response of microbial populations during a field scale bioremediation treatment of chromium contamination. The goal is to generate a training data set for the K-th order logical network model to use.

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Modeling transport and biogeochemical reactions in variably saturated media

Authors: K. Ulrich Mayer

Biogeochemical reactions play an important role in natural and contaminated groundwater systems. Microbial activity controls to a large degree the redox conditions in aquifers and in some cases also in the vadose zone. In addition, biogeochemical reactions contribute to the attenuation of organic and inorganic contaminants and are equally important for groundwater remediation. As a result, multiple reactive transport models of varying complexity have been developed in recent years to help with the interpretation of field and laboratory experiments and to conceptually investigate the role of biogeochemical reactions in aquifer systems. This presentation will provide an overview on formulations and challenges associated with modeling transport and biogeochemical processes in aquifers and the vadose zone. The discussion will be aided by simulation examples from natural attenuation and groundwater remediation studies. Transport modeling in biogeochemically reactive systems requires the integration of advective-dispersive transport, inorganic geochemical reactions, and microbially mediated reactions into a single model. Microbially mediated reactions are of key importance and are often slow in comparison to the time scale of transport, which requires a kinetic representation. In reactive transport models, these reactions have previously been described by Monod or Michaelis-Menten type formulations. More recently, partial equilibrium models have been developed, which assume a two-step process, in which the first step is kinetically controlled, and subsequent reactions are described as equilibrium reactions. Additional approaches of varying complexity have been developed in recent years. Relative merits of these formulations and the comparative ease of integration in reactive transport models will be addressed. Reaction progress and rates of biogeochemical reactions are controlled by the presence of a microbial population and the co-existence and availability of electron acceptors, substrate, and nutrients, which may be present in dissolved, adsorbed or solid state. These reactions can be categorized into a simplified framework: 1) mixing-controlled intra-aqueous reactions, which rely on the mixing of two or more dissolved reactants that are initially present in different regions of the aquifer (e.g. an organic contaminant and oxygen), 2) rate-limited intra-aqueous reactions, which are controlled by the rate of reaction progress in the presence of the essential dissolved reactants (e.g. degradation of an organic contaminant under methanogenic conditions), and 3) rate-limited heterogeneous reactions, in which case the reaction progress is limited by the reactivity of a solid phase (e.g. reductive dissolution of iron oxides). Challenges with parameter determination and implementation into reactive transport models associated with each of these reaction classes will be discussed. Additional challenges with simulating transport and biogeochemical processes in aquifers include temperature dependence of the reactions, the effect of microbial growth and decay, and the production of gases as reaction products. The potential effect of these processes on system reactivity, geochemical evolution, and feedback between flow and transport will also be evaluated.

Multi-level identification of parameterization structure using nonlinear reparameterization

Authors: Inga Berre

Identifying spatial characteristics of porous media reservoirs must in general be based on limited information. We present methodology for identifying the main coarse-scale features of a reservoir based on data with limited information content.

Multi-physics models as a platform for integrated environmental modeling and inverse modeling

Authors: Michael Cardiff, Peter Kitanidis

Environmental problems require models that must simulate a variety of processes across a range of scales. In addition, these models require as inputs parameters that are imperfectly known, and possibly spatially or temporally variable. A simple example of such an environmental problem is the cleanup of light non-aqueous phase liquids (LNAPLs), which requires coupled simulation of both fluid flow and advection/dispersion of the contaminant. Problems such as this are generally "multi-physics", meaning that more than one physical process is simulated. In addition, in order to make useful predictions, these models often require solution of inverse problems (i.e. parameter estimation), which may be highly parameterized and ill-posed. To date, however, most models used in the environmental community are limited to a single physical process or setting, and many do not support efficient inversion strategies. The goal of designing a multi-purpose, multi-domain, and multi-physics environmental model is an admirable one, and one that will require considerable planning and design in order to be met. We hope to contribute to the brainstorming on such a model by analyzing the pros and cons of an existing model, and by drawing attention to the unique facets of environmental modeling that may not be adequately addressed. In this presentation, we discuss our experience with a commercial multiphysics engineering code, COMSOL, and discuss why it may provide a good template for future integrated environmental models. We review COMSOL's strategy for defining and solving coupled, multiphysics models. We also discuss the difficulties encountered when using COMSOL for environmental inverse problems, and present current work on overcoming these obstacles. In general, we conclude that an open-source, freely available multiphysics model would provide a flexible framework that can be tailored to model a variety of physically-based environmental problems. The use of a central multiphysics kernel may also simplify model expansion and encourage the involvement of the community for specific applications.

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Multiphase Flow and Transport Modeling on Different Scales

Authors: Majid Hassanizadeh, Utrecht University and Rainer Helmig, University of Stuttgart

In order to solve complex problems such as CO2 sequestration, NAPL infiltration, or the storage of radioactive waste, multiphysics, multiscale models are indispensible. Often, one can recognize different subdomains for different complex processes, which are governed by small-scale effects. These subdomains require fine resolution. But for comprehensive fine-scale models taking into account multiphase, multicomponent processes as well as heterogeneities in the entire modeling domain, data collection is often far too expensive, and the computational effort is considerable. Therefore, general multiscale, multiphysics concepts are necessary to bridge the gap between various processes and scales.

For this session, we solicit presentations involving new and recent research on theoretical methods that link the molecular with the Darcy scale, as well as research on developing numerical schemes and methods that include multiphase flow and transport at various scales in one solution area. The aim of this research would be to integrate upscaling and numerical methods, such as domain decomposition and multiscale finite volumes, within the advanced framework of multiscale modeling. Contributions that consider applications are also invited.

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Multimodel analysis of pneumatic pressure test data from unsaturated fractured tuff

Authors: Eric Morales-Casique, Shlomo P. Neuman, Velimir V. Vesselinov

We use log permeabilities and porosities obtained from single-hole pneumatic packer tests in six boreholes drilled into unsaturated fractured tuff near Superior, Arizona, to postulate, calibrate and compare five alternative variogram models (exponential, exponential with linear drift, power, truncated power based on exponential modes, and truncated power based on Gaussian models) of these parameters based on four model selection criteria (AIC, AICc, BIC, KIC). As all four criteria favour the first three of these variogram models, we adopt the three favoured models to parameterize log air permeability and porosity across the site via kriging in terms of their values at selected pilot points and, optionally, at some single-hole measurement locations. For each of the three variogram models we estimate log air permeabilities and porosities at the pilot points by calibrating a finite volume pressure simulator (FEHM) against cross-hole pressure data from sixteen boreholes at the site by means of a parallelized version of PEST. Three approaches to calibration are employed: (1) joint estimation of variogram and pilot point parameters based entirely on cross-hole pressure test data; (2) estimation of pilot point parameters based entirely on cross-hole pressure test data, using variogram parameters previously estimated on the basis of single-hole data; and (3) estimation of pilot point parameters based jointly on cross-hole pressure test data and single-hole log permeability measurements, using variogram parameters previously estimated on the basis of single-hole data and a penalty function representing weighted mean squared differences between estimated and measured (prior) log permeability values at coincident pilot point and single-hole test locations, respectively. Assessing the predictive capabilities of each model based on AIC, AICc, BIC and KIC shows a strong preference for one model: exponential when using the first calibration approach and power otherwise. This precludes the use of model averaging for prediction. We therefore use individual models to predict space-time pressure variations during cross-hole tests other than that employed for calibration and validate the predictions against measured pressures. We conclude by assessing the model selection process in light of the validation results.

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Multiscale Thermohydrologic Model Supporting the Total System Performance Assessment for the Proposed Repository at Yucca Mountain

Authors: Thomas A. Buscheck, Yunwei Sun, Yue Hao, Yun Duan, Souheil Ezzedine, Scott C. James

The MultiScale ThermoHydrologic Model (MSTHM) is used in the total system performance assessment (TSPA) for the proposed nuclear-waste repository at Yucca Mountain. The MSTHM uses the Nonisothermal Unsaturated Flow and Transport (NUFT) code to represent thermal-hydrologic (TH) processes occurring at scales from a few tens of centimeters around individual waste packages and emplacement drifts (tunnels) all the way to the kilometer scale for heat flow through the mountain. The MSTHM is used to predict the anticipated range of TH conditions within emplacement drifts and adjoining host rock. To be defensible, the range in predicted TH conditions must address the influence of the variability and uncertainty of engineered- and natural-system parameters that significantly influence those conditions. Parameter-sensitivity analyses show that the most important natural-system parameters are host-rock thermal conductivity and percolation flux through the repository. These analyses show that the key engineered-system parameter is the waste-package-to-waste-package variability in heat output. The range in TH conditions is also influenced by the "edge-cooling" effect, where waste packages closer to the repository edge cool more quickly than those closer to the repository center. To account for this effect, the MSTHM represents the geometric details of the repository layout. Improvements have also been made to how the MSTHM incorporates hydrostratigraphic and percolation-flux data from the Unsaturated Zone Flow Model, which supports ambient flow and transport simulations for TSPA. Other improvements allow more parameter sensitivity cases to be investigated. Twelve cases are analyzed, including four percolation-flux scenarios (10-, 30-, 50-, and 90-percentile) and three host-rock thermal-conductivities (10-percentile, mean, and 90-percentile). Using the results of stochastic analyses, weighting factors are applied to the twelve cases. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract No. DE-AC52-07NA27344. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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NATURAL CONVECTION IN EMPLACEMENT DRIFTS AT YUCCA MOUNTAIN AND IMPACT ON DRIFT SEEPAGE

Authors: Nicholaus Halecky, Jens Birkholzer, George Danko, Davood Bahrami

The heat output from the radioactive waste to be emplaced in the proposed geologic repository at Yucca Mountain, Nevada, will affect the thermal-hydrological (TH) conditions in and near emplacement drifts over a time period of several thousand years. Decay heat will elevate drift temperatures above ambient conditions, establishing temperature and water vapor gradients and subsequent natural convective flows over the drift surface. Formation water in the partially saturated rock mass will evaporate and enter, in the form of water-vapor, the open air spaces of the drift. Vapor will then be transported by natural convection along the drift axis, and will eventually condense in the cold end sections of the drift where no waste is emplaced. This axial transport reduces the moisture content along the heated drift segments, which in turn may affect the potential for formation water to seep into the drift. A new modeling approach was developed for quantifying the in-drift moisture transport processes in emplacement drifts and their impact on drift seepage. A multi-scale modeling procedure solves for the transport of water, water-vapor, air, and heat in both the fractured rock mass and the open air drift, each of which represents a distinctly different flow regime. To fully account for 3D effects, a first model operates on a scale that encompasses the entire drift plus surrounding rock units. In this model, referred to as MF-T2, the flow and transport processes in the rock mass are simulated with the multiphase, multicomponent simulator TOUGH2, and the in-drift heat and moisture flows are simulated with MULTIFLUX (MF), a coupled task solver with a lumped-parameter CFD (Computational Fluid Dynamics) code. MF provides an efficient iterative coupling technique for matching the mass and heat transfer across the boundary between the rock mass and the drift air space. In addition to the full drift-scale model, explicit modeling of the impact of in-drift moisture transport on seepage is being conducted with TOUGH2, simulating a separate high-resolution rock mass model. The necessary drift wall boundary conditions for this model, in-drift temperature and relative humidity, are provided by the full drift-scale MF-T2 model mentioned previously. The new modeling approach has been applied to evaluate the heat-driven flow and transport processes in a representative emplacement drift at Yucca Mountain, embedded in a monolithic, three-dimensional rock mass. Two alternative approaches were tested to simulate in-drift natural convection with the full-scale MF-T2 model: 1) a lumped-parameter CFD dispersion model and 2) a model explicitly modeling the air velocity distribution. Both solution procedures showed good convergence. Our results confirm that the strong natural convection flows predicted by the MF-T2 model, with air velocities of a few centimeters per second, significantly reduce the near-field fracture saturations along heated drift segments, thereby reducing the magnitude of drift seepage.

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New Approach to Reduction of the Dimension of the Reactive Transport Problem

Authors:

The basic problem of real-world reactive transport simulations is too large dimension of the problem given by number of simulated chemical species in solution. Let us omit the discussion on how many dimensions is too much and how many is acceptable - it would be a problem specific classification. The basic approach to solution of such a problem is to classify the solute species to directing and marginal ones. This should be done by an expert-chemist and it can often significantly decrease the problem dimension with preserving accuracy of main phenomena simulation. This approach usually works in case of observation of directing species or conditions influenced by the directing species. If we need to focus on a marginal specie, we can include it into the model and increase the problem dimension. But in situation where all the species are similarly important the dimension reduction obtained this way is not big or the result quality is significantly reduced. We were in such a situation when tried to simulate long-time prediction of contamination transport in Stráž pod Ralskem, Czech Republic after proposed implementation of neutralization in-situ. The underground solution includes 22 measured ions. Some of them are directing the main chemical phenomena and most of marginal ions are dangerous contaminants that should be well observed. In addition the geometric and time size of the problem allows make computation in dimension 3 or 4. It means that the dimension could not be reduced the classical way without massive reduction of result quality. We have proposed an approach of dimension reduction coming from linear algebraic interpretation of the problem. Let us look at the set of all chemical analyses of solutions from the site as the set M of vectors in 22-dimensional linear vector space V with coordinates corresponding to concentrations of individual species. Let us look for such an n-dimensional Vn subspace of V so that M lies “the most close” to it. After identification of the optimal subspace Vn, its suitable basis should be selected. The basis vectors should be interpreted as basic solutions, so all their components should be non-negative and also all coordinates of all members of M in the selected basis should be non-negative. The transport simulations then will be computed in the selected basis and all chemical solutions in the model will be interpreted as linear combinations of basic solutions. Transport phenomena will be simulated the same way as before, just the initial and boundary conditions and outputs should be re-interpreted. The chemical reactions should be interpreted as additional moving of the vectors in Vn and so simulated more carefully. Our contribution deals with proposed approach algorithm, its interpretation and successful results of its application to the above mentioned problem of contamination simulation in Stráž pod Ralskem site.

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New Approaches to Models for the Hydrologic Community

Authors: Larry Murdoch, Clemson University and Venkat Lakshmi, University of South Carolina , and Jay Famiglietti, UC Irvine

Hydrologic models play a key role in both the advancement of hydrologic science and the predictive contributions that hydrology makes to society. Despite their importance, the development of hydrologic models has been far from ideal. Many legacy models are designed with an application focused on a single hydrologic domain (e.g., groundwater, unsaturated zone, rainfall-runoff, channel hydraulics, land surface-atmosphere, wetlands, lakes), which has promoted a compartmentalization of hydrologic thinking and restricted the ability to analyze processes at hydrologic boundaries. Moreover, traditional methods of code development and publication limit the pace at which innovations can be distributed and evaluated by the hydrologic community.

The purpose of this session is to explore new approaches for developing, distributing, publishing, and supporting models for the hydrologic community, and we invite papers addressing this general theme. An example of one such approach is to use data transfer protocols to link together multiple legacy codes, which allows the resulting combination to retain proven capabilities but expand the range of hydrologic interactions that can be simulated. This approach has been used for more than three decades to develop community atmosphere, ocean, land-surface and coupled climate models, and papers describing applications in hydrology are encouraged. An alternative approach is to develop single, stand-alone codes designed to simulate processes across a range of hydrologic domains and scales. Recent advances in computational methods and software have provided a variety of alternatives for simulating multiple hydrologic processes that go beyond the restrictions of single-domain legacy codes. Papers describing these applications are particularly encouraged. We also invite papers describing innovative methods for publishing and supporting models, and allowing the community to interact with models. Models based on open source code are one example of this approach. In addition, Web-based models have made their debut in hydrology, and papers describing this approach for maintaining models would also be well suited to this session.

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New Pore-Scale Analysis for Colloid Filtration Theory

Authors: Kirk E. Nelson, Timothy R. Ginn

Colloid filtration theory (CFT), which has been widely applied to characterize the transport and deposition behavior of both inorganic and microbial colloids in the natural subsurface, is based on a pore-scale analysis of colloid transport in Happel's sphere-in-cell porous media model. The classical CFT analysis assumes that Brownian motion may be treated independently of the other transport mechanisms. Recent studies have indicated this assumption is erroneous. Therefore, a reformulation of the CFT pore-scale analysis is warranted. We present results of a fully Lagrangian methodology for treating all classical CFT transport mechanisms simultaneously. Numerous simulations were conducted over the relevant ranges of parameter values to provide a basis for a new equation predicting the collector efficiency (rate of contact with porous media surfaces) from the various input parameters. Differences with the classical equation (as well as a more recent one based on a fully Eulerian analysis) are highlighted, and a preliminary comparison with experimental data from the literature is presented. Theoretical issues regarding the experimental testing of collector efficiency equations are also discussed.

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Nitrogen Cycle Modeling: Mechanistic Estimate of N-losses From Agricultural Fields on Seasonal Time Periods

Authors: F. Maggi, C. Gu, W.J. Riley, T. Xu, C.M. Oldenburg

The biogeochemical nitrogen cycle and resulting NO2- and NO3- leaching and NO, N2O, and CO2 gas emissions in fertilized agricultural fields are mediated by soil microbial activity, the hydrological cycle, plant dynamics, and climate. Understanding how NO, N2O, CO2 gases and NO2- and NO3- ions are released from agricultural fields to the environment is a key factor in controlling the green-house effect and water contamination, and assumes ever greater importance in view of the foreseen increase in biofuel, food, and fiber production. To address these issues we developed a mechanistic model (TOUGHREACT-N) for various nitrification and denitrification pathways, multiple microbial biomass dynamics, heat and water flows, and various chemical reactions at local and kinetic equilibrium. The soil column is one-dimensional, with hydraulic properties described by a water tension-saturation model. Biotic and abiotic reactions are assumed to follow Michaelis-Menten kinetics, while a consortium of several strains of micro-organisms is assumed to follow multiple Monod growth kinetics accounting for electron donor, electron acceptor, and inhibitor concentrations. Water flow is modeled with the Darcy-Richards equation, while nutrient transport is modeled by Fickian advective and diffusive processes in the aqueous phase and diffusion in the gas phase. Heat flow is modeled with the Fourier equation. Crop dynamics is taken into account by coupling TOUGHREACT-N with CERES to determine water and nutrient uptake, and soil carbon accumulation. TOUGHREACT-N was calibrated against field measurements in several systems to assess pathways of N losses following fertilization. Good agreement between field observations and model predictions was found. We identified two dominant time scales in the system response that depended on plants dynamics. Before plants have substantial impact on soil nutrients and moisture content, N losses are characterized by rapid increases as a function of water application rate and fertilizer amount and application depth. Under reference fertilization and irrigation practices, approximately 1.64% and 1.61% of the total applied N is lost as N-NO(g) and N-N2O(g), respectively, while losses of N-N2(g), N-NO2-, and N-NO3- were several orders of magnitude smaller. When plants grow, pulses in N losses become smoother due to nutrient and water uptake. Contrary to assumptions used in coarse-scale models (e.g., CASA, CENTURY), N losses increase non-linearly with the amount of applied fertilizer and water, and with fertilizer application depth, thus suggesting a revision is in order of long-term estimates of nitrogen and carbon balances at global scales.

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Non-uniform grid coarsening applied on explicit fracture modeling

Authors: Vera Louise Hauge

There is a gap in model sizes between highly detailed geological models (geomodels) with explicit representation of fractures and simulation models used for field-scale studies. Flow patterns are often dominated by large-scale fractures with lengths exceeding a single block in the simulation grid. However, because the fractures are thin relative to their lengths and can have complex geometries, they are difficult to resolve using industry-standard simulation grids. Here we consider two strategies for obtaining simulation models that properly account for the fractures and still have a manageable number of cells. Our starting point is a highly resolved geomodel where fractures are modeled explicitly as grid cells with given permeability and porosity. The first approach generates grids that represent the fractures explicitly also on the coarse grid; we refer to this approach as explicit fracture-matrix separation (EFMS). The second approach is based on a non-uniform coarsening strategy for generating flow-based grids, introduced by Aarnes et al in 2007. We consider a series of two-phase flow simulations to assess the accuracy and the robustness of the two strategies. The numerical results show that the saturations obtained on the non-uniform coarse grids are consistently more accurate than the corresponding saturations obtained by the EFMS method. The numerical results also reveal that it is much easier to tune the upscaling factor with the non-uniform coarsening approach. Finally, we consider extensions to unstructured triangular grids with large-scale fractures with realistic thickness. Necessary modifications to the non-uniform coarsening strategy are considered for the applicability on grids with cells with large difference in volumes.

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Nonequilibrium models of two-phase flow in multidimensions: simulation of gravity fingering and viscous fingering

Authors: Luis Cueto-Felgueroso, Ruben Juanes

The mathematical description of multiphase flow through porous media is still an open problem. The traditional formulation employs a straightforward extension of Darcy's law, which has been used successfully in practice (especially for viscous-dominated, stable flows). It is well known, however, that this extension cannot be rigorously obtained from first principles. At the pore scale, one may delineate different flow regimes, including stable displacement, viscous fingering (diffusion-limited aggregation), and capillary fingering (invasion-percolation). The Darcy-type formulation does not account for the dependence on flow regime, which sets the time scales of displacement processes at the pore level. As a consequence, it is unable to reproduce capillary fingering, viscous fingering, or gravity fingering in multiphase flows. The deficiency of the traditional formulation is particularly noticeable in the simulation of unstable infiltration, in which gravity fingers exhibit saturation overshoot at the finger tip. Several extensions of the traditional formulation have been proposed. These include: (1) the dynamic capillary pressure model of Hassanizadeh and Gray; (2) the hold-back–pile-up model of Eliassi and Glass; and (3) the nonequilibrium model of Barenblatt. What all these formulations have in common is that they include higher-order derivatives in space, time, or mixed space-time. In this paper, we present high-resolution numerical simulations of nonequilibrium models of multiphase flow. The spatial discretization is performed using a rational spectral method or a weighted essentially non-oscillatory (WENO) scheme, depending on the ability of the computational grid to resolve the complex features of the flow. The discretization in time is carried out by a spectral deferred correction method, which is suitable for stiff differential-algebraic equations. These high-fidelity simulations show that advanced continuum models that include higher-order terms are capable of reproducing key features of multiphase flows, including the proper fingering pattern in viscously-unstable flows, and saturation overshoot at the finger tips in gravity-unstable infiltration.

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Novel Block Preconditioners For The Iterative Solution To 3d Large Fe Models Of Coupled Flow-Deformation In Porous Media

Authors: Massimiliano Ferronato, Luca Bergamaschi, Giuseppe Gambolati

The numerical solution of subsurface flow coupled with inelastic porous medium deformation by standard or mixed FE leads to a sequence of linearized symmetric systems with an indefinite saddle point coefficient matrix. Because of the large difference in magnitude between the terms of the flow and structural blocks, the global matrix can be severely ill-conditioned, especially for small time integration steps, with the accuracy of the solution becoming a major computational issue. The selection of an efficient preconditioning technique turns out to be a key factor to accelerate or even to guarantee the convergence of iterative solution methods. A novel block preconditioner, belonging to the class of the so-called constraint preconditioners and denoted as Mixed Constraint Preconditioner (MCP), has been developed for coupled flow-deformation models. The basic idea relies on factorizing the coefficient matrix with the Sylvester\\\'s theorem and approximating such a factorization by appropriate substitutes of the inverse of the (1,1) block and the Schur complement. MCP exploits a twofold approximation of the inverse of the (1,1) block, both implicit and explicit, with the explicit one used to replace the Schur complement. MCP has been experimented with in several realistic 3D applications and compared to more traditional preconditioners, such as an incomplete factorization with partial fill-in (ILUT). MCP with the Symmetric Quasi-Minimal Residual (SQMR) iterative solver may outperform up to five times ILUT in each single time step solution, with even better records over a complete transient simulation. The main reason stems from the fact that a large portion of MCP can be calculated just once at the beginning of the simulation without the need for re-computing at each time step. It is well-known that the use of a lumped capacity matrix in the FE-discretized flow equation helps stabilize the pore pressure solution. Such a procedure, however, typically deteriorates the global matrix conditioning in a coupled flow-deformation model. Numerical experiments provide evidence that this difficulty can be overcome using MCP as a preconditioner. Moreover, MCP proves to be particularly efficient at the initial stage of a transient simulation, where small time integration steps are generally required to obtain an accurate solution. The present communication aims at discussing MCP and its performance in a few 3D large size applications. First, MCP is derived and its main spectral properties outlined. A sensitivity analysis on the parameters required for the preconditioner implementation is performed to provide the user with an indication as to the MCP optimization in different problems. Then, MCP is compared to more traditional preconditioning techniques, with two simplified variants discussed. The results show that MCP appears to be a robust preconditioner for the efficient solution of large size 3D coupled flow-deformation FE models and a quite reliable alternative to more traditional solution techniques. Finally the idea behind MCP can be easily extended to other coupled field problems, such as flow-transport or multiphase flow models, i.e. wherever the FE set of equations possesses a 4-block structure. References: L. Bergamaschi, M. Ferronato, G. Gambolati. Novel preconditioners for the iterative solution to FE-discretized coupled consolidation equations. Comp. Meth. Appl. Mech. Eng. 196: 2647-2656, 2007. M. Ferronato, G. Pini, G. Gambolati. The role of preconditioning in the solution to FE coupled consolidation equations by Krylov subspace methods. Int. J. Numer. Anal. Meth. Geomech., to appear. L. Bergamaschi, M. Ferronato, G. Gambolati. Mixed constraint preconditioners for the iterative solution to FE coupled consolidation equations. J. Comp. Phys., submitted.

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Numerical analysis of pulsed gas injections in respect to oxygen mass transfer and biogeochemical consumption

Authors: Sascha E. Oswald, Gerd U. Balcke

One remediation technique is gas sparging that shall increase the levels of dissolved oxygen in an aquifer and by that enhance biodegradation processes for organic contaminants. However, gas sparging and its effects are difficult to assess, experimentally as well as numerically. We adapted and extended an existing numerical model called KBD, which is based on equations describing the mass transfer processes and gas phase development after injection in a kinetic framework. This model we used to simulate a series of laboratory columns experiments with sandy aquifer material. The experiments included use of a partitioning tracer, measurement of breakthrough curves of dissolved gases and dissolved tracers for a number of oxygen gas pulses. The results showed that the oxygen transfer into the aqueous phase is slowing down with number of pulses of oxygen gas and strongly depends on the reverse transfer and accumulation of nitrogen. Further experiments established a chemical oxygen consuming reaction and proved that the degradation reaction, which depends on the transfer of oxygen into the aqueous phase, itself influences the fate of the gas phase noticeably. Simulations provided a consistent interpretation of the experimental results and spatially resolved data on the composition of the entrapped gas phase, the volumetric changes of the entrapped gas phase and the transport of oxygen through the columns. The numerical analysis then was extended to simulate a field situation of gas sparging including a range of biological degradation rates. In this set-up also differences between injection of pure oxygen versus air were studied. The results give evidence that partitioning tracers and the naturally occurring nitrogen can contribute additional information and the gas dissolution process and thus the transfer of oxygen and the stimulation of biodegradation. The model can be used to better understand the performance of gas sparging set-ups and to assess how biodegradation can benefit from different gas sparging modes of operation.

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Numerical flow and heat transport model of Baños de Brea thermal spring in Galicia

Authors: Javier SAmper, Mercedes BONILLA, José Martins CARVALHO

Construction of a tunnel near the sulphurous Baños de Brea thermal spring in Galicia could affect its flow rate and physical and chemical properties. Its flow rate is 13 m3/day and has a temperature is 22ºC. Thermal spring is located at the contact between metamorphic Ordes Complex and granitic Lalin Unit. Such contact occurs with a regional Normal Fault (Marginal or Pico Sacro Fault) which runs NW-SE (see Fig. 1). Possible hydrodynamic and thermal conceptual models were formulated and their feasibility was analyzed in terms of available data both at the site and from similar thermal areas in Galicia and North Portugal. The most plausible conceptual model assumes that the spring is the discharge of hot waters which infiltrate and flow mostly along the Marginal Fault having about 30 m thickness. Model calibration indicates that a thermal spring can only be explained by the combination of: 1) a high-permeability band associated with a Hercinic fault in granites which has been mapped at the South of the study area and 2) a low-permeability quartz dike located downstream the high-permeability band. This conceptual model was tested with a 2-D vertical finite element groundwater flow and heat transport model. Model results reproduce both flow rate and temperature of Baños de Brea spring and is coherent with common features of thermal systems. Once calibrated the model was used to evaluate the effects of the construction of a nearby tunnel designed for a small hydropower plant. The model takes into account the three phases of tunnel construction: 1) open tunnel, 2) tunnel with concrete grouting and 3) tunnel with final concrete coating. Model results indicate that the construction of the tunnel will affect physical and chemical conditions of the thermal spring neither during its construction nor at the long term.

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Numerical Investigations of the Role of Convective Mixing in Carbon Dioxide Storage in Saline Aquifers

Authors: Keni Zhang, Yushu Wu, Karsten Pruess

When CO2 is injected into saline formations, it partially displaces the resident brine, and partially dissolves in water. Under common subsurface conditions of temperature and pressure, CO2 fluid is less dense compared to water (or brine). The injected CO2 plume will move upward towards the top of saline aquifers and spread out under a low permeability caprock. When CO2 dissolves in brine, the density of the aqueous phase increases by a small amount, 1-2 %. However, the small increase in density may be sufficient to generate significant convection flow in the formation over large times. Previous studies have demonstrated that convection could be much faster than mixing caused by pure diffusion of the dissolved CO2, which accelerates the dissolution of the carbon dioxide. At early times, convection can be initiated on a small scale due to tiny heterogeneity of the formation. Convective mixing processes may generate fingering flow or gravitional instability, which can only be simulated through a high-resolution grid model. In this study, we present a three dimensional numerical model with locally refined mesh to investigate the initial stage of CO2 plume development and plume dilution effects. The time scale taken for the convective instability to begin and grow spatially to encompass the entire permeable interval and permit dissolution of gaseous carbon dioxide is estimated by the model. The influence of vertical permeability, salinity of water, and other rock properties on the development of convective flow is examined. In addition, the intrinsic space scale of the convective process for achieving credible results is investigated using the model. The 3-D large-scale simulations demonstrate that the multi-scale nature of convective mixing can be an important process for the long-term fate of stored CO2 in a brine formation.

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Numerical methods for unsaturated flow with dynamic capillary pressure in heterogeneous porous media

Authors: Son-Young Yi, Malgorzata Peszynska

Traditional unsaturated flow models use a capillary pressure-saturation relationship determined under static conditions. Recently it was proposed to extend this relationship to include dynamic effects and in particular flow rates. In this paper, we consider numerical modeling of unsaturated flow models incorporating dynamic capillary pressure terms. The resulting model equations are of nonlinear degenerate pseudo-parabolic type with or without convection terms, and follow either Richards\' equation, or the full two-phase flow model. We systematically study the difficulties associated with numerical approximation of such equations using two classes of methods, a cell-centered finite difference method (FD) and a locally conservative Eulerian-Lagrangian method (LCELM). We formulate and investigate several variants of the traditional FD using different time splitting schemes and averaging schemes, while LCELM is considered for Richards\' equation with a convection term. The convergence and stability of the methods will be discussed and illustrated. We also discuss the results of our methods for heterogeneous porous media with different rock-types using a full two-phase model.

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NUMERICAL MODEL FOR THE YARQON-TANNINIM GROUNDWATER BASIN, ISRAEL: CHALLENGES AND ADVANCES

Authors: Dafny Elad, Dr. Burg Avi, Prof. Gvirtzman Haim

The Yarkon-Tanninim (YT) groundwater basin, which is the western part of the Israeli Mountain aquifer, is one of the major sources of freshwater in the country. The basin stretches over about 13,000 square km. It is a karstic aquifer of upper Cretaceous, mainly composed of limestone and dolomite. Its eastern part is phreatic, while its western part is confined. The aquifer is stratified, and each layer is somehow heterogeneous due to some facial changes. The aquifer\'s natural outlets were two major springs: the Yarqon ones, adjacent to the city of Tel-Aviv, through which ~225 Million Cubic Meters per year (MCM/y) emerged, and the Tanninim ones, through which ~90 MCM/y emerged. Due to over-exploitation (~400 MCM/y) through hundreds of wells during the last 50 years, the discharge of the Tanninim Springs reduced by about 65% and that of the Yarqon Springs totally dried. At the same time the water levels at the confined part of the aquifer dropped by ~10m. This study aims to numerically model the flow and transport processes in the YT basin. Such a modeling needs to address several challenges such as the complex topography and extreme inclined geology (stratigraphy and tectonics), multiple water tables and lateral shift from confined to unconfined conditions. At the first stage we have comprehensively revised the conceptual understanding of the YT basin, including re-definition of its lateral and bottom boundaries. At the second stage, we have developed a transient, 3D model using the FEFLOW software. The calibration process was very complicated, but very precise, because of the tens of observations points, each of which during tens of years. Thereby, we have established an operational tool for the Israeli Water Authority. The newly developed model will have to face some un-common future operational scenarios, on which we have no past experience, such as: low groundwater levels at a sequence of dry-years; storage of desalinated seawater during winter periods; changing pumping fields due to salination and/or contamination and others. The research is funded by a grant from Israel\'s Water Authority.

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Numerical Modeling of Interactions Among Surface, Vadose Zone, and Groundwater

Author: Jirka Simunek, University of California, Riverside

Hydrologic processes occurring near the land surface, such as precipitation, infiltration, evaporation, transpiration, and runoff, have been historically modeled separately from regional groundwater flow processes. This has been mainly due to large differences in time scales associated with flow within these flow domains. Watershed-runoff models simulate near-surface hydrology in great detail, but greatly simplify or completely neglect subsurface flow. Similarly, regional groundwater models often simplify near-surface hydrologic processes by specifying groundwater recharge based on external calculations independent of groundwater levels. Modeling flow through the unsaturated zone has been a major obstacle to coupling watershed-runoff and regional groundwater flow models. There has recently been considerable effort spent in coupling these independent models, to develop integrated modeling tools that could fully characterize interactions among surface, vadose zone, and groundwater flow.

In this session, contributions are invited that focus on applying and developing new modeling tools that enable evaluation of interactions in complex systems involving surface water, vadose zone water, and groundwater. Contributions may also include studies related to transport of nutrients and various contaminants.

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NUMERICAL MODELING OF A MOUNTAINOUS WATERSHED IN LANYANG CREEK BASIN, TAIWAN USING WASH123D

Authors: Dong-Sin Shih , Gour-Tsyh Yeh

The National Applied Research Laboratories (NARL) in Taiwan is has founded a new national laboratory, the Taiwan Typhoon and Flood Research Institute (TTFRI). The core mission of TTFRI is to conduct research to improve our understanding of natural hazards including typhoons and floods and to abate the lost of lives and properties with earlier warning systems. One of major tasks of the TTFRI is to couple meteorological rainfall model and hydrological watershed model for comprehensively investigating multi hydrological processes in Taiwan. This paper will examine some simulation issues focusing on the watershed scale hydrology. The Lanyang creek basin situated in northeaster Taiwan will be chosen as our study-watershed. We will conduct modeling of hydrology and hydraulics using the numerical model WASH123D. Several land-falling typhoons causing serious disasters were used to calibrate and validate model's parameters. Model conceptualization of coupling 1-D streams, 2-D overland regions, and 3-D subsurface medium will be stated. Calibrations and validations of the model will be presented. The simulation results will be compared with historical data to evaluate model alternatives. Based on this study, it is concluded that the numerical model, WASH123D which is calibrated and validated with measurements, provides a useful protocol for TTERI to conduct research in watershed hydrology.

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Numerical simulation of SIP and NMR responses of coupled pore systems using 3D FEM modelling.

Authors: O. Mohnke, N. Klitzsch, C. Clauser

Structure and state of soils have considerable influence on their flow and transport properties in particular for the vadose zone. The signal responses of both, spectral induced polarization (SIP) and nuclear magnetic resonance (NMR) are sensitive to the inner surfaces of the water filled pore space of soils and rocks. In NMR the evolution of magnetization and in SIP the signal amplitude and phases are related to the size and geometry and surface properties of the pore-matrix system of rocks or soils. Thus, both methods can be applied to derive hydrological parameters such as the hydraulic permeability. Combined numerical simulations of multiphase flow and NMR and SIP responses for isolated and coupled pore systems have been carried out using 3D finite element modelling (FEM) to quantify these relations between measured NMR and SIP signals. These simulations are verified by corresponding laboratory experiments on fully and partially saturated reference samples with accurately defined pore spaces determined by computer tomography (CT). Based on these investigations we aim at an interpretation scheme for combined NMR and SIP measurements in order to assess structure, state and thus flow properties of partially saturated soils.

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Numerical simulation of the far field for a French deep underground repository of long life radionuclides

Authors: Jérôme Jaffré, Estelle Marchand, Jean E. Roberts, Amel Sboui

In France studies for a deep underground repository of long life radionuclides are led by Andra (http://www.andra.fr), the French agency for managing nuclear waste. This is an important multidisciplinary project bringing together hydrogeologists and mathematicians in order to achieve reliable simulations and performance assessment. The French design is based on a three barrier concept, the waste package, the engineered barrier and the geological barrier. Each of these barriers require careful and complex studies. In this talk we will concentrate on the geological barrier and present several difficulties in the numerical methods we encountered and overcame in order to obtain accurate and fast simulations. The location of a possible repository is East of France in a layered sedimentary formation at a depth of about 500m. The mathematical model is simple, with incompressible water flow governed by Darcy\'s law and transport modeled by a linear diffusion-dispersion-advection equation. The domain of calculation representing the far field is of roughly 50 kilometers by 50 kilometers in horizontal extent and 500 meters in depth. It can be divided into 13 homogeneous subdomains. Details can be found in a benchmark at http://gdrmomas.org/presentation.html. The first difficulty lies in the strong heterogeneities since permeabilities, diffusion and dispersion coefficients vary with several orders of magnitude from one subdomain to the other. The second difficulty is that the duration of the simulations is very long (several hundreds of thousands of years). Our method of choice is a cell-cetered finite volume method using the mixed finite element method to calculate the interelement water flow rates and the diffusion-dispersion radionuclide flux. Since a mesh made of difformed cubes was proposed and there was no appropriate mixed finite element for such a mesh we had to construct one and to show that it has the proper approximation properties [1]. For the transport equation we used an upwind explicit scheme for advection, a 1st order implicit scheme for diffusion-dispersion and operator splitting in order to have different time steps for advection and diffusion-dispersion [2]. All these techniques were used for performing deterministic sensitivty analysis based on the SVD decomposition of the sensitivity matrix [3]. Obviously the strong heterogeneities imply different time scales in the various subdomains so we are now implementing a subdomain time stepping based on domain decomposition in space and time. [1] A. Sboui, J. Jaffré, J. E. Roberts, A composite mixed finite element for hexahedral grids, submitted. [2] A. Sboui, Quelques méthodes numériques robustes pour l'écoulement et le transport en milieu poreux, PhD Thesis, Paris-Dauphine university, january 2007. [3] E. Marchand, F. Clément, J. E. Roberts and G. Pépin, Deterministic Sensitivity Analysis for a Model for Flow in Porous Media, Advances in Water Resources, to appear.

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Numerical studies of multiphase flow in porous media

Authors: Doster, Florian, Hilfer, Rudolf

On macroscopic scale, the extended Darcy's theory is currently the most commonly used constitutive theory for multiphase flow in porous media. Problems, however, exists with the description of hysteresis and residual saturations. For example, the capillary pressure and relative permeabilities are usually treated as fundamental parameter functions of the theory although many standard experiments on multiphase flow cleary show that these parameters are process dependent. Possible ways around this problem are to choose different parameter functions related to the particular process one expects. Adjusting the capillary pressure functions according to the corresponding hysteresis path [Lenhard] has been attempted, but is not very useful when the process is not known in advance. Attempts have also been made to formulate a theory starting from elementary physical principles on the porescale. However, as far as we know, none of these approaches leads to a closed set of equations. Here we present some recent results on a constitutive theory for multiphase flow in porous media [Hilfer1] that is based on the insight that percolating and non-percolating fluid parts behave differently, therefore treated as separated phases with distinct constitutive assumptions. Promising results in and near the hydrostatic equilibrium have already been presented earlier [Hilfer2]. This theory is now applied to hydrodynamic regimes. To study the dynamics of systems governed by these equations of motion, we develop an fully implicit finite volume algorithm in one dimension. The numerical studies of test cases like the Buckley Leverett problem, with which we also study the parameter space, are presented. [Lenhard] J.C. Parker, R. J. Lenhard, Water Res. Res. 23, 618 (1987) [Hilfer1] R. Hilfer, Phys. Rev. E 58, 2090 (1998) [Hilfer2] R. Hilfer, Physica A 371, 209 (2006)

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Numerical Studies on Enhanced CO2 Dissolution and Mineral Trapping due to Formation of Aqueous Complexes

Authors: Tianfu Xu, Karsten Pruess

CO2 injected into an aquifer storage reservoir will tend to migrate upwards towards the cap-rock because the density of supercritical CO2 phase is lower than that of water (aqueous phase). In the upper portions of the reservoir, CO2 dissolution into groundwater will lower pH and induce mineral dissolution and complexing with dissolved ions such as Na+, Ca+2, Mg+2, and Fe+2 to form NaHCO3, CaHCO3+, MgHCO3+, and FeHCO3+. Over time these dissolution and complexing processes will increase CO2 solubility, enhance solubility trapping, and will increase the density of the aqueous phase. Aqueous phase will then move downward due to gravity, giving rise to "convective mixing". We have developed a multi-phase reactive geochemical transport model that accounts for the essential processes of flow, transport and chemistry, including changes in aqueous phase density and viscosity due to changes in dissolved species concentrations. Changes in porosity and permeability due to chemical dissolution and precipitation are also modeled. The process of enhanced solubility trapping and convective mixing was explored through application to a gulf coast sandstone saline aquifer. Simulation results indicate that mineral dissolution and formation of aqueous complexes significantly enhance CO2 dissolution and aqueous density. Secondary carbonate precipitation occurs near the CO2 displacement front, resulting in partial self-sealing of the reservoir. This work was supported by the Zero Emission Research and Technology project (ZERT) and by the Director, Office of Science, Office of Basic Energy Sciences of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

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On Leakage of CO2 from an Open Wellbore: Predictions from the Drift Flux Model

Authors: Karsten Pruess

CO2 stored in terrestrial subsurface reservoirs would be buoyant relative to aqueous fluids, and could escape from the primary storage reservoir through natural (faults, fractures) or man-made pathways (wellbores). Depending on fluid pressures, phase composition, and the nature of the flow path, different flow regimes are possible, and different mathematical models may be required to describe the phenomena. In this paper we are interested in two-phase flows of water and CO2 in open pipes, such as improperly abandoned wellbores, for which porous medium-type models are not applicable due to the open nature of the flow conduit. We have adopted the "drift flux model" (DFM) as a convenient approach for describing two-phase flow in open conduits. The DFM includes gravity, friction and acceleration effects and is capable of representing slip between aqueous and gas phases. This paper describes implementation of the DFM into our general-purpose simulator TOUGH2. Exploratory simulations of discharges of water and CO2 from vertical wells reveal a strong tendency towards cyclic and intermittent flows akin to geysering. This work was supported by the Zero Emission Research and Technology project (ZERT) under Contract No. DE-AC02-05CH11231 with the U.S. Department of Energy.

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On Model Selection Criteria in Multimodel Analysis

Authors: Shlomo P. Neuman, Ming Ye, Philip D. Meyer

Hydrologic systems are open and complex, rendering them prone to multiple conceptualizations and mathematical descriptions. There has been a growing tendency to postulate several alternative hydrologic models for a site and use model selection criteria to (a) rank these models, (b) eliminate some of them and/or (c) weigh and average predictions and statistics generated by multiple models. This has led to some debate among hydrogeologists about the merits and demerits of common model selection (also known as model discrimination or information) criteria such as AIC, AICc, BIC, and KIC and some lack of clarity about the proper interpretation and mathematical representation of each criterion. In particular, whereas we [Neuman, 2003; Ye et al., 2004, 2005; Meyer et al., 2007] have based our approach to multimodel hydrologic ranking and inference on the Bayesian criterion KIC (which reduces asymptotically to BIC), Poeter and Anderson [2005] have voiced a strong preference for the information-theoretic criterion AICc (which reduces asymptotically to AIC). Their preference stems in part from a perception that KIC and BIC require a "true" or "quasi-true" model to be in the set of alternatives while AIC and AICc are free of such an unreasonable requirement. We examine the model selection literature to find that (a) all published rigorous derivations of AIC and AICc require that the (true) model having generated the observational data be in the set of candidate models; (b) though BIC and KIC were originally derived by assuming that such a model is in the set, BIC has been rederived by Cavanaugh and Neath [1999] without the need for such an assumption; (c) KIC reduces to BIC as the number of observations becomes large relative to the number of adjustable model parameters, implying that it likewise does not require the existence of a true model in the set of alternatives; (d) if a true model is in the set, BIC and KIC select with probability one the true model as sample size increases, a consistency property not shared by AIC and AICc; (e) published comparisons between BIC and AIC (none consider KIC and few consider AICc) tend to rely on the consistency of BIC, which does not apply when a true model is not in the set; and (f) all four criteria have been used with various degrees of success in such situations. We explain why KIC is the only criterion accounting validly for the likelihood of prior parameter estimates, elucidate the unique role that the Fisher information matrix plays in KIC, and demonstrate through an example that it imbues KIC with desirable model selection properties not shared by AIC, AICc or BIC. Our example appears to provide the first comprehensive test of how AIC, AICc, BIC and KIC weigh and rank alternative models in light of the models' predictive performance under cross-validation with real hydrologic data.

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On Modeling Near-Surface Migration of CO2 from a Shallow-Release Test: Results from the Vadose and Saturated Zones

Authors: Curtis M. Oldenburg, Jennifer L. Lewicki, Laura Dobeck, Lee Spangler

The main challenge facing the geologic carbon sequestration near-surface monitoring community is how to detect small CO2 seepage fluxes that may arise due to leakage from CO2 storage sites. We are carrying out field experiments and simulations using TOUGH2 of near-surface migration of CO2. The field experiments were conceived by the ZERT (Zero Emissions Research and Technology) Project to provide a facility at which researchers can develop capabilities and test approaches for monitoring potential CO2 seepage from geologic CO2 storage sites. The facility located in an alfalfa field adjacent to Montana State University consists of a 70 m-long perforated horizontal well at an average depth of 1.8 m into which CO2 is supplied from a tank for release into six packed-off sections to mimic leakage from a line source such as a fault. The field site is characterized by an organic-rich soil underlain at 1.2 m depth by a sandy cobble with water table at approximately 1.6 m depth. We used observations from a small pre-injection test to estimate effective permeability of the soil and cobble layers at the site. Modeling was used in all phases of the experiment from planning to interpretation. First, simulations were carried out to inform the choice of experimental parameters such as the CO2 release rate, to predict time to breakthrough at the ground surface, width of the seepage zone, seepage flux, and character of the dissolved plume in groundwater below the release zone. After the experiment, simulation results were used to check observations for consistency and to aid in general understanding of the behavior of migrating CO2. TOUGH2/EOS7CA modeling showed that the vadose-zone plume is wider than the surface seepage flux footprint, that CO2 persists in the vadose zone long after the source is turned off and seepage flux stops, that spottiness in seepage flux can arise from subtle effects at the CO2 source, and that when the source is turned on a second time, lag time to breakthrough at the surface is minimal. In the saturated zone, TOUGH2/ECO2N modeling suggested that density-dependent flow due to dissolved CO2 is insignificant, but the dissolved CO2 plume persists over multi-year time scales. This work demonstrates the important role modeling and simulation play in designing field experiments and complementing field data collection and analysis to improve the understanding of subsurface processes. Acknowledgment: This work was funded by the Assistant Secretary for Fossil Energy, Office of Sequestration, Hydrogen, and Clean Coal Fuels, NETL, of the U.S. Dept. of Energy under Contract No. DE-AC02-05CH11231.

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On the Development of Enhanced Geothermal Systems (EGS) with CO2 as Heat Transmission Fluid

Authors: Karsten Pruess, Nicolas Spycher

Recent studies have suggested advantages in operating enhanced geothermal systems (EGS) with CO2 instead of water as heat transmission fluid. For comparable pressure conditions, CO2 was found to achieve heat extraction at larger rates than water. CO2 also has a stronger buoyant drive for wellbore flow, reducing the parasitic power consumption in the fluid circulation system. CO2 is not an ionic solvent, suggesting that it will avoid the strong mineral precipitation and dissolution effects that have caused problems in water-based systems. Finally, while fluid losses in water-based EGS can be a serious problem, losses of CO2 in the subsurface could earn credits for geologic storage of this greenhouse gas. Development of EGS with CO2 would begin with hydraulic and possibly also chemical stimulation, as for conventional water-based EGS. This would be followed by an additional step of reservoir development in which the aqueous phase initially present in the void space in fractures and pores would be removed by circulation of CO2. Removal of water would occur partially by immiscible displacement, and partially by evaporation (or dissolution) of aqueous phase into the flowing CO2 stream. Reservoir engineering studies of EGS with CO2 to date have been limited to fully-developed CO2 circulation systems, as modeling tools were lacking that could describe the entire range of fluid conditions during the development of EGS with CO2. This paper describes a new simulation tool TOUGH2/ECO2H that can treat the entire range of thermodynamic and fluid conditions during the development of EGS with CO2, ranging from near-ambient injection temperatures to 300 oC, and including water-CO2 mixtures ranging from single-phase aqueous to two-phase aqueous-gas to dry anhydrous CO2. The ECO2H fluid property module features a new correlation for partitioning of water and CO2 among aqueous and non-aqueous phases. We present illustrative calculations of the transient evolution of an initially water-based system to an EGS-CO2 upon continuous CO2 injection. The simulations show changes in phase and mass composition as produced fluid changes from aqueous phase initially to two-phase water-CO2 mixtures to single-phase CO2 with temporally declining H2O content. This work was supported by Contractor Supporting Research (CSR) funding from Berkeley Lab, under Contract No. DE-AC02-05CH11231 with the U.S. Department of Energy.

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On the modeling of lignite open pit mine drainage and pit lake filling in a regional groundwater model

Authors: Klauder, Wiebke S., Becker, Bernhard, Schuettrumpf, Holger

On behalf of the federal state North Rhine-Westphalia, three numerical large scale groundwater models representing the geological units “Erftscholle”, “Rurscholle”, and “Venloer Scholle” in the lower Rhine region in Germany have been developed since 1986 till today. The three site specific models cover an area of about 3070 square kilometers and comprise between seven up to nine aquifers with aquitards in-between. The models are based on a transient two-and-a-half-dimensional finite element scheme. Main purpose of modeling is the estimation and forecast of the opencast mine drainage impact on the water balance. With an amount of 565 mio. m³ for the year 2004 for the three opencast mines, the drainage plays an important role for the water management in the region. A substantial part of the modelling deals with the implementation and updating of different boundary condition data. The mine drainage can be modelled with first, second or third order boundary condition type or combinations of them. We discuss the three boundary condition approaches to model opencast mine drainage and show our reasons for selecting the second boundary condition. To create forecasting scenarios and to evaluate the model results efficiently we use a flexible system of pre- and post-processing tools based on database functions combined with advanced data visualization tools. For example we create a spatiotemporal animation, which display the residual hydraulic head for each layer in the open pit mine in order to answer the question, if the particularly area of mining is dry. The opencast mining in the region will end in 2045 and the remediation of the sites includes three pit lakes, but the groundwater replenishment runs until the year 2100. One important question is how much water is needed for the replenishment. Methods for modelling the pit lake filling strategies with a combined set of special boundaries and the evaluation of the results are presented. To deal with large groundwater models needs a convenient system of pre- and post-processing tools. Due to the large amount of boundary condition data, which are often renewed over the years, the combination of database functions and advanced data visualization tools are particularly suitable for modeling the impact of open pit minig on regional water management.

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On the recognition of 20th century climate change in Germany by means of stochastic time-series analysis of regional hydroclimatic data

Authors: Manfred Koch

For Germany, recent regional climate models have predicted significant seasonal changes of, mainly, temperatures and precipitation for the coming century that will require regional adjustments of the management of water resources, particularly, for agriculture. While the average citizen in Germany may have the perceived feeling that climate change, namely, a warming trend with summer extremes has affected the country several times during the last decade - also supported by meteorological measurements - it is still not clear whether such variations are just outliers in the observed hydro-meteorological time series with it's well-known stochastic nature, or whether they are just part of a long-term trend pattern that has already been ongoing over most of the 20th century. As part of a comprehensive study to understand the variability of stochastic hydroclimatic time series techniques, such as the Continuous Wavelet Transform (CWT), Detrended Fluctuation Analysis (DFA) and Singular Spectrum Analysis (SSA) to various hydrometeorological data recorded over most of the 20th century throughout Germany and, namely, within several major river basins. As it is now commonly recognized that the observed variability of such climatic records can be characterized by a nonstationary stochastic process with a few periodic or nearly periodic components acting within time- scales that range from annual, over decadal, centennial to millennial and even longer time periods, the goal is to understand the exact nature of the stochastic process, namely, whether the various observed periodicities are an inherent property of the time series or if they are triggered by external events that act on more or less regular time-scales. Given the maximum record length of ~100 years in the present study, we are able to retrieve periodicities and the degree of persistence - as indicated by the calculation of the Hurst parameter with DFA - acting up to the decadal scale. Cross-correlations of the observed hydroclimatic time series with the North Atlantic Oscillation (NAO) - whose teleconnective effect on the European weather pattern on the inter-decadal scale has been surmised for some time, indicate a strong influence of the NAO on the long-term precipitation, though with somewhat different local effects throughout Germany. Extending the named analysis tools to discharge series in several river basins provides further evidence of such structural breaks in the time-series variability over Germany between the first and second half of the 20th century. While these results can somewhat be taken as indicators of some climate change that has been taking place in this country recently, the abnormal weather conditions experienced here in the last decade may then also be explained more as an inter-decadal intermittency phenomenon rather than as evidence for a long-term climatic trend.

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ON THE UNIFORMITY OF UPLIFT INDUCED BY INJECTING SEAWATER INTO DEEP HYDRAULICALLY HETEROGENEOUS AQUIFERS

Authors: Nicola Castelletto, Massimiliano Ferronato, Giuseppe Gambolati, Carlo Janna, Mario Putti, Pietro Teatini

Recent numerical analyses performed with the aid of advanced hydro-dynamical and geo-mechanical FE models indicate that injecting seawater into a 600-800 m deep brackish aquifer underlying the Venice Lagoon might induce a potential uplift of the city of a few tens of centimetres over 10 years with an important mitigation of the floods that periodically plague Venice. To test the feasibility of an actual full-scale program of anthropogenic Venice uplift, a pilot project in a limited area selected within or in the margin of the lagoon is planned and is ready to be started. A most important issue is concerned with the uniformity of the expected upheaval, an essential requirement for the structural safety of the city historical buildings. Using deterministic simulation models suggested that the predicted uplift was quite uniform all over the Venice area. Both the hydraulic conductivity k and the medium compressibility cM were assumed to be spatially homogeneous within each single geological unit of the litho-stratigraphic sequence forming the Adriatic sedimentary basin. However, a few researchers have disputed the assumption of the homogeneity with regard to k, thus implying a possible influence of the k spatial distribution on the predicted city uplift. The present communication addresses the issue of the hydraulic heterogeneity of the injected formation and how it relates to the uniformity of the differential land displacements. The study is performed with the aid of an uncoupled modeling approach, i.e. solving first the saturated subsurface flow equation and then using the resulting over-pressure as a source of strength in a poroelastic FE model. A Montecarlo approach is used to determine the PDFs of both horizontal and vertical components of the ground displacement. An appropriate number of stochastic realizations of a log-normal isotropic stationary random k are generated on the basis of information available from several exploratory boreholes of the Northern Adriatic basin. The influence of uncertainties in the stochastic distribution of k values is tested by means of a sensitivity analysis in which specific knowledge of the basin genesis and evolution is considered. The results of the simulations are used to evaluate the risk of exceeding a given displacement gradient threshold. Two values are considered for this threshold: 5x10-4 (0.5 m over 1000 m), i.e. the bound normally required for the safety of buildings; and 4x10-5 (0.04 m over 1000 m), i.e. the differential anthropogenic land subsidence experienced by Venice over the period 1961-1969, and that resulted in no destructive effects on the stability of the constructions. The results of the present preliminary investigation indicate that, because of the beneficial smoothing effects of the overburden, the above limits are never reached in the city area irrespective of the properties of the assumed k statistics.

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On the Upscaling of the reaction-advection-diffusion equation in porous media with monod-like kinetics.

Authors: F. Hesse, F. A. Radu, M. Thullner, S. Attinger

The contamination of groundwater is a severe problem in many industrial and developing countries as it imposes a severe threat to water resources. Therefore the biodegradation of these groundwater contaminants has been extensively investigated in the laboratory and in the field. However, a direct quantification of in situ biodegradation is often impossible. The extrapolation of laboratory results on microbial degradation processes to in situ biodegradation processes in the field is challenged by finding an adequate description of the bioavailabilty of chemical species. In porous media, microorganisms are primarily residing on the surface of the solid matrix. Thus, their activity is controlled by species concentrations in their immediate vicinity, only. Controlled by transport processes at the pore or sub-pore scale these bioavailable concentrations differ from average concentration measured at the macro-scale. We investigate (bio)reactive transport processes within individual pores or pore assemblies. By explicitly resolving pore geometries, advective-diffusive transport and microbial degradation are simulated by making use of the software toolbox UG allowing for a quantitative analysis of bioavailabilty limitations on microbial contaminant degradation. These numerical simulation results are accompanied by analytical upscaling leading to the formulation of effective equations with effective degradation and effective leading to the formulation of effective equations with effective degradation and effective dispersion coefficients for biodegradation processes at the pore scale. We will demonstrate that, in addition to the classical result of a reaction- and a diffusion-limited regime in case of first order degradation processes, a new transition regime appears for Monod kinetics. The new regime indicates a concentration limitation (this phenomenon is known from lab experiments). The three regimes and their implications for practical applications are discussed.

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Optimal water and gas injection strategies for CO2 storage in depleted oil reservoirs

Authors: Tara LaForce

In CO2 storage in depleted oil reservoirs it is of critical importance to maximize the reservoir volume containing CO2. Injecting water simultaneously with CO2 in aquifers has been shown to increase the volume of CO2 that can be stored as a trapped phase because injected water inhibits the ability of CO2 to rise under buoyancy forces, allowing more of the aquifer depth to be utilized. In an oil reservoir, a similar result is likely. Moreover, if there are active wells in the reservoir then injection of water will prevent early production of CO2. We use analytical solutions for a one-dimensional model to study a variety of simultaneous water and gas injections strategies for a reservoir containing a mixture of light and heavy hydrocarbon components with and without water. The model accounts for three-phase flow of four components through a porous medium and uses a cubic equation of state to model gas/oil phase behavior. In oil reservoirs super-critical CO2 may generate a multi-contact miscible displacement of remaining hydrocarbons, so both miscible and immiscible injection of CO2 is studied. We consider the implications of using CO2 in order to improve oil recovery, and find that this is often a competing goal with storing CO2 far from production wells. –Mixtures which create efficient miscible displacements result in earlier breakthrough of injected CO2, while mixtures that have delayed arrival of CO2 in production wells have less favorable oil recovery.

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Optimization Problems in Hydrology

Author: Stefan Finsterle, Lawrence Berkeley National Laboratory

This session will focus on computational methods and their application to various hydrological optimization problems, including (1) parameter estimation by automatic model calibration (inverse modeling), (2) optimal design of testing and monitoring systems, and (3) optimization of water resources management and remediation operations. Common to all these optimization problems is the need to minimize some objective function by adjusting certain model parameters that represent hydrologic properties, the system layout, or operational variables. The objective function may measure the misfit between calculated and observed data, actual (and/or penalty) costs, and other quantifiable objectives; it may also include various regularization terms. A large number of global and local algorithms have been proposed to map out or minimize potentially nonconvex, nonlinear, or noncontinuous response surfaces in high-dimensional, usually constrained parameter spaces. Successful solution of a hydrological optimization problem requires careful parameterization of the problem, choosing an appropriate objective function, and selecting a robust and efficient minimization strategy. We seek contributions that address these optimization challenges by discussing the overall approach as well as algorithms and computational issues. We also welcome case studies that demonstrate the usefulness and limitations of mathematical optimization in hydrology.

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Optimizing Model Calibration and Water Resource Management Strategies Under Uncertainty: New Approaches and Findings

Authors: Barbara Minsker, Abhishek Singh, Shenquan Yan, Douglas Walker, Albert Valocchi

Prediction models are often coupled with optimization methods to aid in model calibration and identifying management strategies for monitoring or remediation. Identifying optimal solutions that are robust to prediction uncertainty is challenging, particularly for computationally-intensive models and incorporating subjective information. This talk will discuss two promising new approaches to address these challenges: dynamic surrogate modeling and interactive calibration under uncertainty. The first approach aims to reduce computational cost, which is a critical issue for large-scale water resource optimization problems when multiple simulations are required to evaluate objective function values over parameter realizations. The dynamic surrogate modeling approach adaptively approximates and replaces time-consuming prediction models within a noisy genetic algorithm (GA) optimization framework. The surrogates are trained to predict the distribution of the objectives online, using Latin Hypercube simulation results created and archived during the GA run. The surrogates are then adaptively updated to improve their prediction performance and correct the GA's convergence as the search progresses. The GA is modified to incorporate hypothesis tests to produce reliable solutions. The second new approach addresses uncertainty assessment for model calibration using an interactive multi-objective genetic algorithm (IMOGA) that considers subjective user preferences in addition to quantitative calibration measures such as calibration errors and regularization. Predictive uncertainty analysis for the IMOGA consists of a multi-level sampling approach, incorporating uncertainty in both large-scale trends and the small-scale stochastic variability in parameter fields. The multiple solutions found by the IMOGA are considered alternative models of the large-scale structure of the parameter field. Small-scale uncertainty is considered to be conditioned on the large-scale trend and correlated with a specified covariance structure. The prediction model is run using all simulated fields to obtain the distribution of predictions, which are then combined using model averaging approaches such as GLUE (generalized likelihood uncertainty estimation) and MLBMA (maximum likelihood Bayesian model averaging). Both of these methods are applied to field-scale groundwater remediation case studies and the results show significant improvement over more traditional methods.

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Parallel Coupled Watershed-Nearshore Model Development

Authors: Robert M. Hunter, Jr., Jing-Ru C. Cheng, Hwai-Ping Cheng, Tim Campbell

The U.S. Army Engineer Research and Development Center (ERDC), together with the Naval Research Laboratory (NRL), is working to couple the Parallel Watershed Flow model (pWASH123D) and the parallel Advanced Circulation model (ADCIRC). pWASH123D is a first-principle, physics-based numerical model to simulate a coupled system of one-dimensional (1-D) channel networks, 2-D overland regimes, and 3-D subsurface media. ADCIRC is a finite element hydrodynamic model for coastal oceans, inlets, rivers, and floodplains. The coupling of the two models is being achieved through the Earth System Modeling Framework (ESMF). This work is a task in the Battlespace Environments Institute (BEI) that is sponsored by the Department of Defense High Performance Computing Modernization Program (DoD HPCMP). The BEI aims to migrate existing DoD models and simulation tools of climate/weather/ocean modeling and simulation, environmental quality, and space weather models to the ESMF. ESMF consists of an infrastructure of utilities and data structures for creating model components and a superstructure for coupling them. Developed for the Earth science community, ESMF was initially designed to support models that incorporate structured grids (unstructured support is currently in development). Both pWASH123D and ADCIRC utilize unstructured meshes for model simulation. To provide unstructured mesh support, the use of the ERDC's DBuilder library in conjunction with the ESMF has been incorporated to perform the coupling of the two models. The DBuilder is a parallel data management library written primarily for unstructured mesh models. The coupling of the two models requires three distinct phases. Phase one is startup of the applications under the same Message Passing Interface environment. This is accomplished through the ESMF. Phase two consists of determining shared nodes/elements between the meshes of the two models. Many models do this as a preprocessing step, but the coupling of pWASH123D and ADCIRC will incorporate this feature at runtime through the use of the DBuilder library. Phase three is data exchange between the models. Both the DBuilder library and the ESMF will be used for the implementation of the data exchange. This presentation will discuss the methodologies used to couple unstructured independent models through ESMF and DBuilder. It will also show the scalability of the coupled model. Two examples, one of which performs hypothetical flow simulations in the area of Biscayne Bay coastal wetlands and oceans in south Florida, will demonstrate the different results between uncoupled and coupled models. The coupling allows ADCIRC to provide "improved" boundary conditions for the watershed model, and vice versa. This research generates a tool to better manage water resources in an estuary watershed.

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Parameter estimation of stochastic flow and transport models for the design of groundwater monitoring networks

Authors: Jessica V. Briseño Ruiz, Graciela S. Herrera

The main objective of groundwater monitoring networks is to carry out assessments of groundwater heads and contaminant concentrations and their variation over time. In the design of this type of networks, a method that involves space and time in a combined form was proposed by Herrera (1998). The method uses a Kalman filter coupled with a stochastic flow model. The advantage of the stochastic model is that it estimates the model predictions uncertainty, which allows recognizing areas that have large uncertainty, making the methodology effective in the selection of sampling well positions and sampling times that reduced the uncertainty estimation. When applying this method it is important that the stochastic characteristics of the model be congruent with field data, but in general it is laborious to get a good match between them by hand. For these reason, the main objective of this work is to apply a Kalman filter to achieve parameter estimation using a priori space-time covariance matrix obtained from the stochastic model. The method consists of three steps: (1) Given the mean and semivariogram of the hydraulic conductivity (K) and the natural logarithm of K (ln K), realization of these parameter are obtained through sequential Gaussian simulation. (2) Using each K realization, the stochastic flow model is solve to produce a realization of hydraulic head (H) and concentration (C), to obtain the prior mean H and mean C estimation and its covariance matrix. (3) Given a prior estimation and the corresponding covariance matrix, the ln K parameter estimated is obtained using the Kalman filter. The synthetic study case presented is based on a simplified representation of the Queretaro Valley aquifer in Mexico. The results indicate that the errors of the parameter estimation generated with the filter are congruent with the confidence intervals predicted by the theory.

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Peclet-dependent memory kernels for transport in heterogeneous media

Authors: Andrea Cortis

Transport in heterogeneous media can be described by partial differential equations, which exhibit convolutions with time and/or space memory kernels. In this work, we characterize the full time spectrum of time-memory kernels by applying a nonparametric inversion algorithm to macroscopic synthetic data for heterogeneous porous media, Our findings put into evidence the inherent nonuniqueness of the transport parameters for nonlocal transport models. Notably, we find that the Péclet number can be interpreted as an ancillary parameter of a family of probability distribution functions that characterizes the memory kernels of transport.

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POD Calibration for ADH

Authors: Corey Winton

We are solving inverse problems in groundwater modeling. Given values of hydraulic head at discrete locations, we seek to approximate values of hydraulic conductivity for the entire field. We are using ADH, a finite element code developed at the Coastal & Hydraulics Lab in Vicksburg, MS. When using ADH to model large, complex groundwater behavior -- for instance the entire state of Florida -- extreme run-times prohibit the frequent function calls needed for parameter estimation. Proper Orthogonal Decomposition (POD) is a method to reduce the size of the problem to calibrate ADH, reducing the number of full function calls needed. We will introduce the problem, discuss POD and how it is used for steady-state problems, and demonstrate the accuracy of the POD solution compared to the full ADH solution.

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Pore-Scale Reactive Transport Modeling and Upscaling To the Continuum Scale

Authors: Peter C. Lichtner, Los Alamos National Laboratory and Qinjun Kang, Los Alamos National Laboratory

Multiphase flow and reaction in porous media are among the most complex and challenging problems in water resources research. Although pore-scale interfacial phenomena govern the key processes of fluid mobility, chemical transport, adsorption, and reaction, spatial heterogeneity at the pore scale cannot currently be resolved at the continuum scale, where averaging typically occurs over length scales larger than typical pore sizes. An open question is how important spatial heterogeneity at the pore scale is for the observed behavior at the larger scale. Specifically, resolving pore-scale heterogeneity may explain some of the discrepancy between lab-measured and field-derived rate constants, as well as other issues leading to failure of macroscale models. Therefore, to quantitatively investigate how pore-scale heterogeneity affects the emergent behavior at the field scale, we must understand multiphase flow, transport, and reaction processes at the pore scale. When combined with upscaling techniques, pore-scale simulations may enable the key parameters and physiochemical processes that control macroscopic phenomena to be identified, and the most appropriate continuum model to be determined, or even to demonstrate whether upscaling is impossible. In cases where upscaling is shown to be valid, pore-scale simulations can provide appropriate values for macro-scale properties of the porous medium, including primary and secondary flow domains and interfacial area, permeability, tortuosity, and dispersivity.

This session will be devoted to recent advances in this area and will include: (1) more accurate representations of porous media, such as direct imaging, statistical reconstruction, and process-based modeling; (2) different methods to simulate multiphase flow and reactive transport in porous media at the pore scale, including lattice-Boltzmann, pore-network, and smooth-particle hydrodynamic methods; and (3) different approaches to upscaling pore-scale results to the continuum scale. Applications of these methods to subsurface contaminant migration, bioremediation, geological CO2 sequestration, etc., are particularly sought.

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Pore Scale Simulation of Multiphase Flow through Fractures in Porous Media

Authors: Lateef Akanji , Stephan Matthai

The flow of immiscible fluids through natural fractures in a porous rock matrix is controlled by pore- and fracture geometry, fracture aperture and fluid and capillary pressure gradients. While much work has been done on flow in fractures in non-porous materials, there is a lack thereof for porous media fractures. Commonly, two-phase flow in fractures is modelled using a relative permeability saturation relationship, kri(sw). Originally, this formulation included a flow rate-dependency (e.g. Barenblatt 1960) which currently is largely ignored in spite of considerable evidence for it (e.g Fourar et al 1993, Chen et al. 2004). Furthermore, cross terms in the original formulation suitable for a consideration of the viscous drag among flowing fluid phases are also usually neglected although experimental data show otherwise (e.g. Fourar and Lenormand, 1998). In this work, I will develop a first principle-based numerical simulation method based on a discrete representation of both fractures and pore space. This will eventually allow to place new constraints on fracture kri by making it possible to analyze separately the flow in the matrix and fracture void space. My work in progress has thus far validated a two-dimensional pore scale model for the case of single phase flow, including automatic determination of pore diameter, maximum pore capillary pressure and saturation distribution. This has already allowed me to estimate effective permeability and capillary pressure curves from thin section micrographs and micro-CT scan of selected porous media. Future work is now being directed at describing the interplay of multiphase flow processes in complex heterogeneous fractured porous media. Citations: Barenblatt 1960, Basic Concepts in the Theory of Seepage of Homogeneous Liquids in Fissured Rocks (Strata) PMM Vol 24 852-864; Chen et. al. 2004, Experimental study of liquid-gas flow structure effects on relative permeabilities in a fracture WRR 40 W08301 doi:10.1029/2004WR003026, Fourar et al. 1993, Two-phase flow in smooth and rough fractures: Measurement and correlation by porous-medium and pipe flow models, WRR 29, 3699-3708. Fourar and Lenormand (1998): A Viscous Coupling Model for Relative Permeabilities in Fractures. SPE 49006 (254-258).

Pore scale simulation of multiphase fluid flow and reactive transport using particle methods and continuum fluid dynamics.

Authors: Paul Meakin, Hai Huang, Alexandre Tartakovsky, Zhijie Xu, Xiaoyi Li

Pore scale simulation of multiphase fluid flow and reactive transport using particle methods and continuum fluid dynamics. Paul Meakin1,2,3, Hai Huang1, Alexandre Tartakovsky4, Zhijie Xu1 and Xiaoyi Li1 1. Idaho National Laboratory, Center for Advanced Modeling and Simulation 2. Physics of Geological Processes, University of Oslo 3. Multiphase Flow Assurance Innovation Center, Institute for Energy Technology, Kjeller 4. Computational Mathematics Technical Group, Computational & Information Sciences Directorate, Pacific Northwest National Laboratory During the past two decades pore network and lattice Boltzmann models have provided the primary approach to the simulation of multiphase fluid flow in fractured and porous media at the pore scale. More recently, particle models such as smoothed particle hydrodynamics (SPH) and dissipative particle dynamics, as well as continuum grid-based computational fluid dynamics combined with interface tracking/capturing and dynamic contact angle models have been developed and applied to multiphase fluid flow and reactive transport. These models (pore network, lattice Boltzmann, particle and continuum) have complementary strengths and weaknesses, and multiphase fluid flow cannot yet be accurately and reliably simulated for all geologically relevant fluids and conditions. Recent progress towards the goal of developing broadly applicable models for multiphase fluid flow and reactive transport, with a focus on SPH and grid-based continuum methods will be presented. Different approaches to including phase separation in SPH models (particle-particle interactions, two-phase equations of state and Ginzburg-Landau free energy functionals) will be briefly discussed and the strengths and weaknesses of several interface tracking/capturing methods (volume-of-fluid, level set, particle level set and phase field) that are being applied to multiphase fluid flow and reactive transport simulations will be presented. Current pore scale modeling and simulation capabilities will be illustrated using examples from our own work and the work of others. Finally, the potential impact of the next generation of high performance computers on the simulation of multiphase fluid flow and reactive transport in porous media, fractures and fracture networks will be discussed.

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Pore-scale modeling of reactive and non-reactive transport: Upscaling and multiscale hybrid modeling

Authors: Timothy D. Scheibe, Alexandre M. Tartakovsky, Bruce J. Palmer, Marshall C. Richmond, Yilin Fang, Brian D. Wood

Pore-scale simulations of flow, transport, and reactions in porous media (in which the geometry of solid grains and pore spaces is explicitly quantified) are being used to demonstrate links between microscopic processes and macroscopic phenomena. Pore-scale models are often used to develop understanding of fundamental processes that can then be incorporated into larger-scale models (e.g., darcy-scale) that treat porous media as effective continua. We are exploring two approaches in parallel: 1) direct upscaling of pore-scale simulation results using volume averaging methods, and 2) multiscale hybrid modeling, in which multiple models defined at fundamentally different length and time scales (e.g., pore and darcy-scale models) are combined within the same overall spatial and temporal domain. We have developed pore-scale simulation capabilities using a particle-based (mesh-free) smoothed particle hydrodynamics (SPH) approach as well as a grid-based finite volume computational fluid dynamics (CFD) approach. We will present results that explore upscaling of model results and model hybridization with emphasis on the following: a) cross-validation and comparison of pore-scale models using SPH and CFD methods, b) upscaling of dispersion parameters in realistic pore geometry, c) coupled flow, transport and mineral precipitation in a solute mixing zone, and d) computational performance and multi-processor scalability of pore-scale model codes.

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Pore-Scale Modeling of Transport in Charged Porous Media

Authors: Partha P. Mukherjee, Qinjun Kang, Peter C. Lichtner

Transport involving multicomponent, multiphase flow and reaction in porous media is among the most important and challenging problems in water resources research. Although pore-scale interfacial phenomena govern the key processes of fluid mobility, chemical transport, adsorption, and reaction, spatial heterogeneity along with charge conservation of surface complexation reactions at the pore scale is unresolved in the continuum reactive transport models involving averaging over length scales much larger than typical grain sizes. To represent these processes mathematically requires formalism for local diffusive processes between the bulk fluid and the charged mineral surface. However, continuum formulations as currently employed cannot account for local concentration gradients at mineral surfaces and fail to address the influence of intricate pore-scale processes, leading to a lack of fundamental understanding of the underlying physics of transport and reaction in the sub-micron and micron length scales. In this work, a comprehensive pore-scale modeling framework for investigating transport in the presence of charged mineral surface in porous media based on the mesoscopic Lattice Boltzmann (LB) method is developed to account for electric double layer effects on transport in single aqueous phase, multicomponent systems and the implication of such study in energy and environmental systems is elucidated.

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Pore-scale Simulation of Dispersion Using Discontinuous Galerkin Finite Element Method and Random-Walk Particle Tracking

Authors: Sreejith Pulloor Kuttanikkad, Christian Engwer, Peter Bastian, Kurt Roth

Fundamental understanding of solute transport through porous media has immense importance in many natural and industrial processes such as groundwater remediation, chromatography and nuclear waste disposal. However, accurate modeling and simulation of solute transport through porous media still poses a great challenge to researchers due to the complexity of pore-spaces. Pore-scale modeling is generally accomplished by network modeling approach or direct numerical simulation. Network modeling approach, though widely used, generally over-simplifies the complex pore geometries. On the other hand, Direct numerical simulation using classical numerical methods requires a grid resolving the complex pore-spaces. In practice, creating such a mesh is a highly involved process and hence structured grid based methods are most appealing for pore-scale modeling. One such a method, based on Discontinuous Galerkin finite element method has been developed in our group. We apply the above approach to simulate the flow and transport in porous media at the pore-scale. We are interested in computing macroscopic parameters such as dispersion coefficients from pore-scale simulation and in particular, to study their dependence on complex pore-scale geometry. We solve Stokes equation, which governs the laminar, incompressible and viscous flow through porous media at the pore-scale using the above approach to obtain the pore-scale flow field. We then simulate transport using a Lagrangian based random-walk particle tracking approach. We will show three-dimensional pore-scale flow and corresponding hydrodynamic dispersion through a random packing of impermeable spheres. The particle tracking method can be implemented with much efficiency because the flow field is computed on a structured grid. We will study the asymptotic behavior of solute dispersion for a wide range of Peclet numbers and compare our results with various experimental and numerical results from literature.

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Pore Scale Simulation of Multiphase Flow through Fractures in Porous Media

Authors: Lateef Akanji, Stephan Matthai

The flow of immiscible fluids through natural fractures in a porous rock matrix is controlled by pore- and fracture geometry, fracture aperture and fluid and capillary pressure gradients. While much work has been done on flow in fractures in non-porous materials, there is a lack thereof for porous media fractures. Commonly, two-phase flow in fractures is modelled using a relative permeability saturation relationship, kri(sw). Originally, this formulation included a flow rate-dependency (e.g. Barenblatt 1960) which currently is largely ignored in spite of considerable evidence for it (e.g Fourar et al 1993, Chen et al. 2004). Furthermore, cross terms in the original formulation suitable for a consideration of the viscous drag among flowing fluid phases are also usually neglected although experimental data show otherwise (e.g. Fourar and Lenormand, 1998). In this work, I will develop a first principle-based numerical simulation method based on a discrete representation of both fractures and pore space. This will eventually allow to place new constraints on fracture kri by making it possible to analyze separately the flow in the matrix and fracture void space. My work in progress has thus far validated a two-dimensional pore scale model for the case of single phase flow, including automatic determination of pore diameter, maximum pore capillary pressure and saturation distribution. This has already allowed me to estimate effective permeability and capillary pressure curves from thin section micrographs and micro-CT scan of selected porous media. Future work is now being directed at describing the interplay of multiphase flow processes in complex heterogeneous fractured porous media. Citations: Barenblatt 1960, Basic Concepts in the Theory of Seepage of Homogeneous Liquids in Fissured Rocks (Strata) PMM Vol 24 852-864; Chen et. al. 2004, Experimental study of liquid-gas flow structure effects on relative permeabilities in a fracture WRR 40 W08301 doi:10.1029/2004WR003026, Fourar et al. 1993, Two-phase flow in smooth and rough fractures: Measurement and correlation by porous-medium and pipe flow models, WRR 29, 3699-3708. Fourar and Lenormand (1998): A Viscous Coupling Model for Relative Permeabilities in Fractures. SPE 49006 (254-258).

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Preconditioning Newton-Krylov methods for reactive transport

Authors: Laila Amir , Michel Kern

Modelling reactive transport in a porous medium has important applications to areas like bioremediation in polluted sites, nuclear waste storage simulations, and CO2 sequestration studies. When local chemical equilibrium is assumed, we are led to a system of advection-diffusion PDEs coupled with algebraic equations. In this context, the role of the chemical solver is simply to separate mobile and immobile parts of each species. In a recent work [ ], we investigated a fully coupled approach, formulated in terms of total mobile and immobile concentrations for each component. Its main advantage is to keep the chemical code distinct from the transport code, in contrast to the direct substitution method. The proposed approach leads to a huge non-linear system that has be solved by some variant of Newton method. In a large scale situation, computing the Jacobian, let alone factoring it, may not be feasible because of the storage requirements. We have thus chosen to use a Newton-Krylov method, also called Jacobian-Free Newton method, where the linear system arising at each Newton iteration is solved by an iterative method like GMRES. This avoids the necessity of forming an explicit Jacobian matrix, and only requires the ability to form the product of the Jacobian by a given vector. As this is a directional derivative, it can be computed exactly or approximated by finite differences, so that the actual Jacobian elements are never explicitly needed. In our context, we have found that computing exactly the Jacobian-vector product (as opposed to using finite differences) is essential for efficiency. This is possible provided we can compute the Jacobian of the chemical solver (which is a small matrix). Recent work [ ] has shown that it is possible to solve efficiently geochemical problems using Newton-Krylov methods, but finding a efficient preconditioning still remains a major issue. Since no actual matrix is available, a preconditioner has to be matrix free. Due to our choice of unknowns, the Jacobian has a natural block structure, reflecting the different unknowns in the system. We first show how (linearized) operator split solvers can be used as preconditioners. We also investigate the relationship between such decoupled solvers and block Gauss-Seidel preconditioning. A second step keeps more terms of the original matrix in the preconditionedr, by computing an (approximate) Schur complement. A further refinement is to try and improve the convergence of Newton\\\'s method by nonlinear preconditioning [ ], that seeks to replace the original nonlinear system by an equivalent nonlinearly preconditioned system whose nonlinearities are more balanced. We validate our approach on the numerically difficult “MoMas Reactive Transport Benchmark” (see http://www.gdrmomas.org/ex_qualifications.html#geochimie). References - Amir, M. Kern, Newton-Krylov methods for coupling transport with chemistry in heterogeneous porous media, submitted to Computational Geosciences, 2008. - G. E. Hammond, A. J. Valocchi, and P. C. Lichtner, Application of Jacobian-free Newton--Krylov with physics-based preconditioning to biogeochemical transport, Advances in Water ressources, 28:359--376, 2005. -X.-C. Cai and D. E. Keyes, Nonlinearly preconditioned inexact Newton algorithms, SIAM J. Sci. Comput., 24:183-200, 2002.

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Predictability experiments with a river flow ensemble forecast system

Authors: Dingchen Hou, Kenneth Mitchell, Zoltan Toth, Helin Wei

Hydrologic processes such as stream flow are strongly coupled with atmospheric processes related for example to precipitation and temperature. Since the atmosphere is a chaotic system with limited predictability, hydrologic predictability is limited not only by our ability to simulate the natural (and human induced) hydrologic processes, but also by the loss of information that is captured at initial time in the estimate of the state of the coupled atmosphere / land surface system due to the dynamical growth and eventual nonlinear saturation of forecast errors. In such a situation, ensemble forecasts offer a practical tool to predict the future state of the coupled system in a probabilistic fashion, potentially leading to more complete and informative hydrologic forecasts. Through experiments with the NCEP Global Ensemble Forecast System (GEFS) coupled with the Noah Land Surface Model (Noah LSM), this study analyzes how various aspects of a coupled atmosphere / land surface forecasting system supports and limits river flow forecasting. The role of initial conditions, numerical models, and ensemble-based uncertainty estimates for the atmospheric and land surface components, including human induced processes (river regulation) will be discussed on river flow predictability, with an emphasis on the limitations of atmospheric ensemble forcing.

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PREDICTING THE PERFORMANCE OF GEOTHERMAL RESERVOIRS: SOME USEFUL NUMERICAL TECHNIQUES

Authors: George Zyvoloski, Rajesh Pawar

Geothermal Energy has been used for centuries for space heating. It has been used for decades for electrical power generation. With the growing interest in carbon free power generation and it's relatively low cost, geothermal energy is likely to become an important resource in the future. Determining the resource potential of new and existing reservoirs will require numerical models that can accurately predict future reservoir performance including the requisite subsurface physics capability to simulate fracture growth and dilatation in low permeability rock. Accurate prediction of reservoir performance depends on a validated numerical model and a thorough understanding of uncertainties associated with the model. In this talk we will describe several numerical impediments to accurate simulations of future geothermal reservoir performance, namely, inadequate grid resolution and lack of appropriate physics, and present some solutions. In field scale simulations, a compromise between adequate grid resolution and computation time is often difficult to achieve. The level of required grid resolution depends strongly on the use of the model, the data used in calibration, and the type of prediction desired. A reasonable level of grid refinement can be determined a priori. Bower et. al. (2000) studied the effect of grid resolution on numerical models where the hydrostratigraphy as well as the flow changed with grid size. Their results showed that an acceptable grid size could be found by calculating flow and transport on a sequence of grids with simple (prescribed hydraulic heads) boundary conditions and representative permeability values. They identified an acceptable grid size as one in which the bulk flow through the grid changed very little from the next coarser grid. In this talk, a similar approach will be applied to a hypothetical geothermal reservoir that includes several hyrdogeologic units and faults and realistic boundary conditions. Using a very fine grid synthetic model as "truth", the determination of an "adequate" grid will be made in a manner similar to Bower et. al (2000). After establishing an "adequate" grid size, the model will be calibrated using the automated calibration code PEST. The calibration parameters (permeabilities) will be compared to the very fine grid synthetic model parameters. The calibrated coarse grid model will be used to predict future reservoir performance and the predictions will be compared to that of the very fine grid model. The management of geothermal reservoirs usually requires drilling new wells to optimize reservoir performance. Traditional approaches of re-gridding around wells, based on the existing grid resolution, flowrates, and other parameters in a numerical model, can greatly increase simulation time due to resulting large number of gridblocks. We will evaluate applicability of a new numerical tool (the embedded wellbore model (EWM) to address the near-wellbore resolution problem. The EWM module basically embeds a high resolution wellbore into a coarse grid without a need for regridding or grid-refinement (as required by other wellbore incorporation approaches). In contrast to analytical approximations to radial flow in gridblocks, the formulation is independent of the subsurface physics. Highly fractured geothermal reservoirs often experience thermal short-circuiting from injection wells to production wells. The ability to simulate this phenomenon, often influenced by the thermal contraction of the rock surrounding fractures, requires the coupling of geomechanics with heat and mass transfer. This can lead to computationally intensive simulations. We will examine several numerical formulations, from relatively simple pore pressure based models to those with fully coupled thermal, hydrologic, and mechanical coupling and compare them on their ability to predict reservoir performance within the combined constraints of adequate grid resolution and process realism.

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Prediction of Aleatoric and Epistemic Uncertainty

Authors: Metin M. Ozbek, James L. Ross, George F. Pinder

The characterization of uncertainty in hydrological systems has traditionally been accomplished using probability theory. This paper addresses the growing need in hydrological systems modeling and management to segregate uncertainty, whether it occurs in input parameters or in possible alternative models for the system, into aleatory uncertainty and epistemic uncertainty. Aleatory uncertainty is also referred to as variability, irreducible uncertainty, stochastic uncertainty and uncertainty due to chance whereas epistemic uncertainty is commonly referred to as reducible uncertainty, subjective uncertainty, and uncertainty due to lack of knowledge. Our objectives are 1) the modeling of both types of uncertainty within the unifying framework of random sets, and 2) the development of new algorithms that will yield simulation results in a computationally efficient manner and accurately propagate both uncertainties. An application of our approach to groundwater flow and transport modeling at the Woburn, MA site will evaluate its computational efficiency and accuracy over a purely probabilistic approach as well as a well-known approach to propagate epistemic uncertainty.

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Prediction of Groundwater Quality Changes in Response to CO2 Leakage from Deep Geological Storage

Authors: Liange Zheng, John A Apps, Yingqi Zhang, Tianfu Xu, Jens T Birkholzer

If carbon dioxide stored in deep saline aquifers were to leak into overlying aquifer containing potable groundwater, the intruding CO2 would lower groundwater pH and could enhance the solubility of hazardous inorganic constituents present in the aquifer minerals. As an effort to evaluate risks associated with geologic sequestration of CO2, this work assesses these potential effects using reactive transport modeling. A systematic geochemical evaluation of more than 38,000 groundwater quality analyses from aquifers throughout the United States provided the prerequisites for reactive transport modeling. For example, galena (under reducing conditions) and cerussite (under oxidizing conditions) control aqueous Pb (lead) whereas arsenopyrite component in pyrite controls aqueous As (arsenic) generally under reducing conditions. Reactive transport simulations are performed which focus on the chemical evolution of Pb and As in the groundwater after the intrusion of CO2. The simulations use representative mineralogies for shallow potable aquifers in the USA and two measured mineralogies for deep confined aquifers. The resulting concentrations of Pb and As in the groundwater are then compared to the EPA specified health- based limits for drinking water. A significant increase of aqueous Pb and As occurs, although in most situations they remain below health-based limits. Sensitivity studies are also conducted for variation in hydrological, geochemical and mineralogical conditions and several critical parameters. The results indicate that aquifers containing more carbonate (through pH buffer) and clay minerals (by adsorption) are less vulnerable to CO2 intrusion. Adsorption/desorption from minerals surface significantly impact the mobilization of Pb and As. Adsorption dampens the effect of galena and arsenopyrite dissolution by removing Pb and As from aqueous phase under reducing conditions. Under oxidizing condition desorption is primarily responsible for increasing the concentration of aqueous Pb while precipitation of cerussite downstream stabilize aqueous Pb concentration.

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Production Capacity Assessment: Case-Study Svartsengi

Authors: Jonas Ketilsson, Gudni Axelsson, Halldor Palsson, Magnus Thor Jonsson

In this study a deterministic modeling approach is developed for the general numerical simulation of geothermal resources, for assessment of production capacity, addressing both sustainability and reversibility. The simulator iTOUGH2 (i.e. Inverse modeling of Transport Of Unsaturated Groundwater and Heat) is used, for which comprehensive pre- and postprocessor have been designed. The processors facilitate the creation of discrete irregular grids, visualization of physical conditions and visualization of convective pore velocities in the reservoir. The postprocessor also compares observed field data with the transient model response, showing both absolute and residual values. The simulator iTOUGH2 is used for optimization of selected parameters, which minimizes the residual of the observed and calculated response. A sensitivity and error analysis is essential if the parameter estimation is to be performed because a good match does not necessarily mean that the estimates are reasonable. They may be highly uncertain due to high parameter correlation, which is usually an indication of over-parameterization. The case study of the Svartsengi geothermal system in Iceland shows how effective the model approach is in simulating the transient physical condition. The parameter estimation was effective in matching the observed pressure drawdown, temperature and enthalpy of the produced fluid. The predicted response of Svartsengi in 2007-2037, for a 560 kg/s production rate (~70 MW e) with 120 kg/s injection, caused the physical conditions to be unfeasible after two decades. However, the current rate of 360 kg/s production (~50 MW e), with 120 kg/s injection, appears to be sustainable for the next three decades. A recovery period following the production scenarios studied indicates that initial pressure in the reservoir will be reached in 2100-2140, although initial reservoir temperature will not have been recovered. The present study underestimates the production capacity of the two-phase zone and therefore the total production capacity of the system is likely to be higher than predicted. How detailed a model of a geothermal system must be, to possess reasonable predictive capabilities, is not known at present. More complex models of geothermal systems, using a well-by-well approach, introduce a greater degree of freedom, so that problems of solution uniqueness may arise. However, the intrinsic weakness of the more simple volumetric method, used in the 1985 Iceland national geothermal resource assessment, is the fixed recovery factor, while energy recovery strongly depends on the recharge, physical conditions and properties of the reservoir. Thus, the present modeling approach is a possible alternative to the earlier model approaches. Its main advantage is that it takes into account the key physical conditions and properties of geothermal resources. This model approach can therefore be used for a future national reassessment of geothermal resources in Iceland.

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Pumping Optimization of Coastal Aquifers based on Evolutionary Annealing-Simplex

Authors: George Kourakos, Aristotelis Mantoglou

Management of coastal aquifers involves complex evaluations using computationally intensive numerical models such as SEAWAT. When these models are integrated into an optimization framework based on global optimization algorithms (simulated annealing, Genetic algorithms, etc.), the overall computational time may be exceptionally large. The present study develops an alternative methodology based on a heuristic Evolutionary Annealing-Simplex Scheme (EASS), where a generalized downhill simplex methodology is coupled with a simulated annealing procedure to perform the optimization search. In order to reduce the computational burden, dispersion in the costal aquifer is simulated using Artificial Neural Networks and training is carried out simultaneously with optimization in an iterative manner. As optimization progresses, the weights and biases of the network are adjusted so that the network performs well in the current search space. Combining EASS with ANN, results in a near-optimum solution using a relatively small number of function evaluations of the numerical model (SEAWAT). In cases with many decision variables, training of a network may be computationally intensive and a division of the master network into smaller sub-networks is used to train the network. Using this approach, it is possible to train only parts of the networks that do not perform well. The proposed EASS-ANN scheme is evaluated in three applications and compared to three global optimization algorithms (Genetic Algorithm Simulated annealing, threshold acceptance). Two hypothetical applications with 4 and 13 decision variables respectively were useful for performing sensitivity analysis on crucial parameters and configuring the algorithm (initial population, training schedule, radius of influence and neural network structure). The optimum configurations were applied in a real application in the coastal aquifer of the Greek island of Santorini. The results show that the proposed EASS-ANN scheme performs equally well as other well known global optimization techniques and requires significantly less computer time.

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Quantifying microbial activity in subsurface environments using stable isotopes as biogeochemical tracers

Authors: Andrew Dale, Pierre Regnier, Doug LaRowe, Jose Mogollon

Earth scientists are increasingly attracted by the unique potential of numerical models which are able to resolve, in time and space, the complex interplay between mass transport, chemical reactions and geomicrobial processes. This is particularly true in subsurface porous environments, such as aquatic sediments, where chemical fluxes are often constrained by the activity of well-defined microbial communities. In many ecosystems, low levels of microbial activity appear to be the rule rather than the exception, which adds a challenging dimension to detecting and quantifying key biogeochemical processes where analytical methods are unsuitable or unavailable. However, because micro-organisms in natural environments tend to be fussy consumers, they often fractionate metabolites taken into the cell during growth, leaving behind a subtle isotopic fingerprint in the medium or in their cellular biomass. Reactive transport models which can explicitly account for low microbial activity levels in addition to distributions of isotopes thus prove to be extremely useful and sensitive tools for analysing and quantifying chemical fluxes arising from microbial activity. In this communication, the underlying concepts behind reactive-transport modelling of stable isotopes in subsurface systems hosting energy-limited microbial communities will be presented and supported by applications relevant to the Earth sciences.

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Reactive Percolation using Pore-Network Modeling

Authors: Lionnel Algive, Samir Bekri, Olga Vizika-Kavvadias, Mostafa Fourar

Paper Description : Dissolution and deposition modeling is crucial to ensure geological CO2 sequestration. In carbonate reservoirs particularly, the CO2-induced acidification causes the matrix dissolution near the wellbore. The ionic species may further reprecipitate and form deposition layers, either because of incompatible water mixing, or due to variations in thermodynamic conditions. Consequently, the potential permeability decrease could reduce the economically accessible volume and ultimately lead to the project rejection. The aim of this work is to develop a numerical tool, based on pore-network modeling (PNM), that describes the effects of a reactive flow on transport properties and structure evolution at the core scale. The model is based on the resolution of the macroscopic convection-dispersion equation for a reactive solute. Its coefficients, namely apparent volumetric reactive coefficient, mean solute velocity and dispersive coefficient, are analytically calculated, for each unit cell of the network, by solving microscopic equations and using upscaling techniques. The deposit location and thickness and their impact on petrophysical properties (permeability-porosity relationships) are determined as functions of rock characteristics and reactive flow regimes. Results : It has been observed, numerically and experimentally within glass micromodels, that the deposit map depends both on microscopic and macroscopic scales through relevant dimensionless numbers, Peclet and Damköhler, defined at the appropiate scale. Depending on the values of these numbers, the deposition occurs, at pore scale, either uniformly, in throats or in pores, whereas, at core scale, it takes place along the main flow paths or uniformly. It was found that the corresponding K-Φ laws are different from the Cozeny-Karman law that is usually used in reservoir simulators. A such arbitrary function is deficient to describe dissolution-deposition phenomena. The main advantage of this work is to provide constitutive K-Φ laws, based on a physical description, to be used as input in reservoir simulators to enhance CO2-storage performance predictivity.

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Reactive transport analysis of microbiological zoning in groundwater flows

Authors: Craig M. Bethke, Dong Ding, Qusheng Jin, Robert A. Sanford

Reactive transport modeling helps explain the origin of the microbiological zoning observed in pristine freshwater aquifers. Zoned aquifers have been described previously as either thermodynamic or kinetic phenomena, but neither interpretation has proved fully satisfactory. Drawing on concepts of population dynamics, the modeling reported here offers an alternative explanation of how certain microbes exclude others from zones: one functional group maintains conditions under which cells in another group die more rapidly than they can reproduce. The modeling also lends support to the idea that a group of microbes that appears to dominate a particular zone in an aquifer may in fact coexist with, or even be subordinate to another group.

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Regional and Site-Scale Modelling in Support of a Proposed Deep Geologic Repository in Canada for Low and Intermediate Level Radioactive Waste

Authors: Jonathan F. Sykes, Eric A. Sykes, Stefano D. Normani, Yong Yin, Young-Jin Park, Edward A. Sudicky

A Deep Geologic Repository (DGR) for Low and Intermediate Level radioactive waste has been proposed by Ontario Power Generation for the Bruce Nuclear site in Ontario Canada. The DGR is to be constructed at a depth of about 680 m below ground surface within the argillaceous Ordovician limestone of the Cobourg Formation. The objective of this paper is to develop regional-scale and linked site-scale geologic conceptual model for the DGR site and to describe flow system evolution using the FRAC3DVS-OPG flow and transport model. This provides a framework for the assembly and integration of site-specific geoscientific data that explains and illustrates the influence of conceptual model, parameter and scenario uncertainty on the predicted long-term performance of the geosphere barrier. The modelling also provides a basis for planned investigations of the DGR, serves as a basis for exploring potential anthropogenic and natural perturbations to the DGR system, and demonstrates the long-term stability of the deep system. In the geologic framework of the Province of Ontario, the Bruce DGR is located at the eastern edge of the Michigan Basin. Well logs covering Southern Ontario have been used to define the structural contours at the regional and site scale of the 37 sedimentary strata that may be present above the Precambrian crystalline basement rock. The regional-scale domain encompasses an 18,500 km2 region extending from Lake Huron to Georgian Bay. While the selection of a larger domain might decrease the impact of boundary-condition uncertainty on site-scale performance measures, it significantly increases the contribution of the far-field uncertainty in the spatial characterization of the geology, especially when extrapolating strata geometry to the model boundaries where data are sparse. The site-scale spatial domain encompasses an area of approximately 19 km by 19 km with the repository at its centre. Its boundary conditions are determined from the regional scale analysis using the traditional nested model approach. An alternate approach involves the use of sub-gridding. From a hydrogeologic perspective, the domain can be subdivided into two horizons: a shallow zone characterized by the units of the Devonian and a deep zone comprised of the low-permeability units of the Silurian and Ordovician and the more permeable Cambrian where present. The deep groundwater zone is characterized by units containing stagnant water having high concentrations of total dissolved solids that can exceed 300g/l. Hence, the conceptual model of the Bruce DGR site required the development of constitutive models that relate the fluid density and viscosity to the fluid composition (e.g. TDS and major ions), temperature and pressure. The computational sequence involves the calculation of steady-state density independent flow that is used as the initial condition for the determination of pseudo-equilibrium for a density dependent flow system that has an initial TDS distribution developed from observed data. Long-term simulations that consider future glaciation scenarios must also include heat transport and change-of-state (e.g., permafrost formation and thaw). Sensitivity and uncertainty analyses can be computationally intensive, particularly for large-scale dynamic problems that couple energy, flow and mass transport. The analyses are therefore evolutionary, beginning with a sensitivity study to isolate key parameters postulated to be most important. Also important in the sensitivity and uncertainty analysis is the selection of the performance measure used to evaluate the system. The traditional metric of average water particle travel time is inappropriate for geologic units in which solute transport is highly diffusive. The use of life expectancy and groundwater age is a more appropriate metric for such a system. The mean life expectancy for the DGR and base case parameters has been estimated to be in excess of 10 million years.

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Regional evaluation of changes in potential evapotranspiration under a changing climate and influences on recharge and runoff

Authors: Alan L. Flint, Lorraine E. Flint, Justin L. Huntington

The influences of climate change scenarios on potential evapotranspiration (PET) were investigated using a regional scale model for the 5 states in the southwestern U.S. PET was calculated at 270-m grid spacing using an hourly model that relies on solar radiation modeled using topographic shading and cloudiness and was done on a 20-node homemade Beowulf Cluster. PET was calculated using 2 different formulations, Priestley-Taylor and Hargreaves-Samani. The model was calibrated using stations calculating reference evaporation (California Irrigation Management Information System, CIMIS; The Arizona Meteorological Network, AZMET; The Pacific Northwest Cooperative Agricultural Network, AGRIMET) throughout the study area. Comparisons between the 2 formulations were in good agreement with the reference stations (which are on relatively flat terrain) but differ in mountainous terrain where solar radiation on slopes (which is not explicitly included in the Hargreaves-Samani approach) is highly variable. Potential climate change scenarios were represented using the International Panel on Climate Change A2 and B1 Scenarios, the Geophysical Fluid Dynamics Laboratory model (GFDL), and the National Center for Atmospheric Research's Parallel Climate Model (PCM). When the increase in air temperature approaches 3 C there is generally an increase in potential evapotranspiration (about 10 percent), but the amount of increase is highly variable over the southwestern US. The resultant increase in potential evapotranspiration leads to a general decrease in recharge (about 4 percent) and runoff (about 8 percent) but the decreases are highly variable spatially. These reductions were enhanced due to a decrease in snow accumulation and early spring snow melt.

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Representing the biosphere in a reactive transport model of wastewater reuse

Authors: Gretchen R. Miller, Yoram Rubin, K. Ulrich Mayer

Reuse of wastewater through land application for irrigation or groundwater recharge has become a common practice in water-stressed areas. In California's Central Valley, approximately 500 food-processing facilities use this method to dispose of their wastewater, which is commonly high in salts, nitrogen compounds, and labile organic carbon. In many cases, land application is the sole method of wastewater treatment, and natural attenuation is expected to prevent degradation of the underlying groundwater. The processes associated with this degradation include: plant uptake in the rooting zone, microbially mitigated redox reactions such as denitrification and respiration, cation exchange, and mineral dissolution and precipitation. In this work, we use the multi-component reactive transport code MIN3P to describe the physical and biological vadose zone processes associated with the waste application, evaluate the relative contributions of each process to overall waste attenuation, and estimate breakthrough concentrations of nitrogen, organic carbon, and fixed dissolved solids (FDS) at the water table for several scenarios. In order to incorporate the conceptual model into the existing numerical code, we integrate information from several disciplines, describing the biogeochemical reactions with parameters drawn from the literature on constructed wetlands and natural attenuation of hazardous waste, and deriving root solute uptake rates from logistic nutrient accumulation functions found in the agronomy literature. The model simulations indicate that the biosphere and its control over the nitrogen-carbon-oxygen (N-C-O) system may be highly influential over salinity attenuation. The model suggests the potential for a strong connection between carbon dioxide production, from biodegradation and plant roots, and salinity levels reaching the groundwater table, especially under moderate to high soil saturation conditions. The interaction between biodegradation and soil physical processes is also important to predicting nitrogen breakthrough; in some cases, the simulations indicate that sorption dramatically slows ammonium breakthrough, delaying it by up to 30 years. This paper demonstrates the necessity of including multiple plant, soil, and microbial processes as well as a suite of chemical components in models of wastewater reuse, in order to capture the complexity of their interactions.

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Review of Optimization Methods for Parameter Estimation and Experimental Design in Groundwater Modeling

Authors: William W-G. Yeh

This paper reviews optimization methods used for parameter estimation and experimental design in groundwater modeling. The inverse problem of parameter estimation seeks to identify the parameter structure as well as the corresponding parameter values using input and output observations. Once the distributed parameter is properly parameterized and objective function and constraints properly formulated, the problem can be solved by algorithms developed in nonlinear programming, such as the gradient-based Gauss-Newton algorithm; or the global search algorithms, such as the genetic algorithm (GA). This paper also discusses the various parameterization methods, the computation of the Jacobian matrix, and the combined use of local and global algorithms. Experimental design deals with the selection of a set of experimental conditions such that a specified criterion is optimized. The optimization is subject to a set of constraints. The experimental conditions include the number and location of pumping/recharge wells, the number and location of observation wells, the pumping/recharge rates, and the sampling frequency. This paper reviews the classical criteria derived from statistics for experimental design and various algorithms used for solving the inherent combinatorial optimization problem.

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Risk Analysis for Leakage in Geological CO2 Storage Considering Large Database Reservoir Statistics

Authors: Kopp Andreas, Binning Philip, Johannsen Klaus, Class Holger, Helmig Rainer

Carbon dioxide sequestration is a promising technology for managing anthropogenic carbon dioxide fluxes into the atmosphere where CO2 is stored in subsurface reservoirs. The engineering design of a carbon dioxide sequestration system is subject to considerable uncertainty. For example, there is some chance that geological conditions will lead to leakage from the CO2 reservoir. In order to select suitable geological formations for CO2 sequestration and design these systems it is therefore important to develop a concept of risk. This work develops a novel risk assessment framework for CO2 sequestration by investigating CO2 plume evolution in a reservoir using numerical simulations based on a large statistical database of potential CO2 reservoir properties. There are many ways that risk can be defined. Risk is usually defined in terms of three questions: How can a system fail? What is the likelihood of failure? What are the consequences of failure? The evaluation of these questions is difficult because of the lack of data, poor knowledge of processes, etc. The consideration of all possible scenarios is an impossible task. Therefore comprehensive studies of risk analysis relies on expert opinions to judge the most appropriate methods for evaluating risk (Oldenburg, 2007). Here a first attempt at defining a simple method for evaluating risks in CO2 sequestration is presented. One way in which a CO2 reservoir can fail is by leakage through fractures, wells or other geological weaknesses located at some distance away from the CO2 injection well. Leakage is judged to be significant if it occurs within a given time period. Such a failure can be evaluated numerically using the sophisticated multiphase-multicomponent non-isothermal reservoir simulator MUFTE_UG. The simulator is used to determine the distribution of CO2 in the reservoir, and failure is defined to occur if the CO2 has spread a given distance away from the injection point at a given time. This is equivalent to stating that reservoirs where the CO2 is spread over a greater lateral area are more risky than reservoirs with a compact CO2 volume. The second part of risk assessment is to determine the likelihood that such a failure will take place. This can be assessed by considering the potential range of reservoir parameters like permeability, porosity, depth, geothermal gradient etc. These were determined from a database including information from over 1200 reservoirs. Based on this data, probability density functions (pdf\'s) have been derived. The parameter space of potential reservoir properties can then be sampled and simulations conducted to assess the distribution of CO2 in the subsurface. For each simulation, failure is assessed by examining whether CO2 has spread to a given radius within a given time. As many simulations are required to cover the parameter space, this is a computationally demanding task. In order to complete the required simulations, the project used the \'CO2 Community Grid\' environment by the Nordic Data Grid Facility. The final part of a risk assessment is to determine the consequence of failure, or the damage. In this paper, damage is defined to be equivalent to the mass of CO2 leaking out of a reservoir. Here the leakage mass is defined to be the total amount of CO2 spreading past a given radial distance away from a well at a given time. While the concept of risk defined in this paper is very simple, it is intended to provide a systematic framework for engineers to determine the ideal properties for a CO2 sequestration reservoir. The paper presents the results of such a risk assessment and provides recommendations for the type of reservoirs that should be considered for sequestration systems. Bibliography: C.M. Oldenburg, Screening and ranking framework for geologic CO2 storage site selection on the basis of health, safety, and environmental risk. Environmental Geology, DOI 10.1007/s00254-007-0947-8, 2007.

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Robust Multi-D Transport Schemes with Reduced Grid Orientation Effects

Authors: Jeremy Kozdon, Brad Mallison, Margot Gerritsen

The grid orientation effect (GOE) is a phenomenon which leads to the computation of fundamentally different solutions on grids oriented at different angles to the principal flow direction. This phenomenon is most significantly seen in adverse mobility ratio flow simulations when the injected fluid is much more mobile than the resident fluid, as in gas injection problems. Due to an underlying physical instability at the simulation scale, numerical results are highly sensitive to discretization errors and hence the orientation of the underlying computational grid. Though there are many errors made in any simulation project, the advective transport errors are amongst the most critical for GOE. One of the primary factors is the grid dependent form of the diffusive numerical error terms. In this work, we examine the role of numerical diffusion in triggering undesirable modes, and use our improved understanding to design a new upwind discretization scheme for transport that reduces GOE. We consider truly multi-D finite difference and finite volume methods and restrict our attention to first order upwind schemes. We begin by using modified equations analysis to predict preferential flow directions on structured grids for several popular schemes. For miscible displacement problems which involve linear advective transport, the discretization schemes should be positive to prevent nonphysical overshoots and oscillations in the concentration field. However, straight forward extensions of multi-D schemes to transport in heterogeneous porous media characterized by rough velocity fields do not maintain positivity. Therefore we develop an interaction region based framework appropriate for arbitrary grid topologies for which local and robust positivity constraints can be formulated, even for highly heterogeneous media. The previously analyzed multi-D schemes are also formulated within this framework so that they are appropriate for porous media. Within this framework it is possible to begin with a multi-D upwind scheme and add a corrective flux so as to design a scheme with a “minimal” constant amount of transverse (cross-wind) numerical diffusion: large enough to reduce GOE, but small enough to allow fingering to be triggered by variations in physical parameters, such as rock permeability and porosity. We call this new scheme the Flat-scheme. Extensions to second order accuracy within this framework are also discussed. We use two miscible gas injection test problems to demonstrate the value of truly multi-D schemes: (i) the homogeneous quarter five-spot problem with two different orientations of the grid with respect to the principal flow direction and (ii) a radial injection into both homogeneous and heterogeneous media. For both tests truly multi-D schemes, and in particular the Flat-scheme, greatly reduce grid orientation effects and numerical biasing compared to dimensional upwinding.

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Robust numerical methods for modelling non-isothermal and multiphase reactive transport of CO2 storage

Authors: M. A. Sbai

This presentation gives an overview of the modelling concepts developed in the framework of a general purpose multi-component and multi-phase reactive transport model targeted for numerical studies of CO2 sequestration. Fluids mass and energy balance equations are coupled with reactive transport of primary chemical components in the aqueous, mineral, and gas phases. The numerical solution technique is fully implicit in time, and combines finite element and finite volume space discretisation techniques in space. The system of nonlinear sparse algebraic-differential equations is solved using an adaptive Newton-Raphson iteration embedding a semiautomatic control of time step refinement or coarsening. During this iterative process, a dynamic reduced degree of freedom algorithm enables significant reduction in computational requirements, global matrix assembly, and memory storage for long term safety assessment of CO2 sequestration sites. For instance, a two-phase and three-component system composed from heat-water-CO2 is effectively solved as an isothermal two-phase, two-component, water-CO2 system when temperature changes are the least significant. Reactive transport equations are formulated assuming the thermodynamic local equilibrium assumption in the aqueous phase, and kinetic reactions in the multi-component gas, biological, and mineral phases. Aqueous, immobile, and gas components are chosen as the system primary dependent variables, while the secondary dependent variables are free-ion aqueous component concentrations and aqueous complex concentrations. The solution method adopted for the nonlinear coupled equations is a hybrid version of the global implicit procedure. It enables switching from the most accurate, but the highest in terms of computational burden, one step solution technique, to the lowest order sequential iteration method, which is the most in common use nowadays. This selective coupling procedure enables to easily drop, or tightly couple, a set of chemical components from the system Jacobian by acting on their cross-derivative entries in the reaction rate terms. Benchmark and numerical studies representative of the fundamental processes of (i) the dissolution of CO2 gas phase in a deep saline aquifer, (ii) the convective instability created by density gradients between the rich CO2-aqueous solution and the initial aqueous solution are presented to demonstrate the simulator capability to tackle problems associated, but not-limited, to performance analysis of long-term storage. These studies have led to identification of several characteristic time scales, associated to gas diffusion in the aqueous phase, capillarity trapping by immobilizing the residual CO2 mass fraction, the convective dissolution, and cross-diffusion mechanism regime when the convective instability dies at late times. The role of physical heterogeneity on enhancement or dissipation of the convective instability phenomena is further illustrated through two specific applications to a revised geological model of the Sleipner saline aquifer (North-Sea, Norway), and to the Dogger aquifer, which is a candidate for CO2 storage in Paris basin (France). Acknowledgment: This research work is supported by the French Agency for Scientific Research (ANR), under contract number ANR-06-CO2-006-01 in the framework of Heterogeneities-CO2 project.

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Root-Soil Interactions

Convener: Jan W. Hopmans, University of California Davis

Root surfaces represent one of the most important phase boundaries in nature, since most mineral nutrients essential for life enter the biosphere and the food chains of the animal world through the roots of higher plants. Similarly, root water and nutrient uptake is one of the most important processes considered in numerical models simulating water content and fluxes in the subsurface, thus controlling water flow (recharge) and nutrient transport (leaching) to the groundwater, and exerting a major influence on predictions of global climate models. In addition to soil transport mechanisms, nutrient uptake is controlled by the spatial distribution of roots, as influenced by its architecture, morphology, and presence of active sites of nutrient uptake, including root hairs.

In this special section, we seek original contributions that advance theory and modeling of root-soil interactions, as determined by a wide number of environmental variables, including atmospheric forcing, moisture, nutrient and other stresses, and that include root water and nutrient uptake processes. We especially seek examples across a wide range of spatial scales, including the global scale, and advances in numerical approaches that couple flow and transport in the presence of roots, and that include experimental data.

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Modeling Radionuclide Transport with First-order Chain Reactions

Authors: Yunwei Sun, Steve F. Carle, Mavrik Zavarin, Gayle A. Pawloski

Radionuclide decay and in-growth are usually described as first-order chain reactions. Modeling of reactive transport coupled with those chain reactions becomes computationally expensive, even impossible, when the number of radionuclides is large or stiff reactions are involved. In order to facilitate the simulation of chain reactions, flow and transport processes are often simplified. Sometimes, when transport is focused, the chain reactions have to be treated as unrelated species while the in-growth is ignored. The system of first-order radioactive decay chains in a batch reactor can be expressed analytically by the well-known Bateman equation. When transport in a realistic system (heterogeneous and anisotropic system with species-dependent retardations) is coupled with those chain reactions, we develop Bateman-type closed-form solutions to simplify the coupled chain reactions without losing the decay and in-growth nature. All tests in the Rainier Mesa/Shoshone Mountain Corrective Action Unit at the Nevada Test Site were detonated in the unsaturated zone of Tertiary volcanic tuffs. Simulating transport in this hydrogeologic setting involves multiphase and multiple coupled species, and thermal processes, and should not be simplified as single-phase advection with steady-state flow. To assess transport implications for the total radionuclide inventory, we prefer to describe the transport in details and to decouple chain reactions analytically. Operator Splitting (OS) is often used for solving partial differential equations of advection-dispersion-reaction (ADR) systems. Each operator can be solved separately using an algorithm appropriate to its mathematical behavior. Although a lot of research has been done in operator-splitting for solving ADR equations, numerical approaches for the reaction operator are computationally expensive. To meet the convergence criteria of ODE (ordinary differential equation) or DAE (differential algebraic equation) solvers, a transport time step has to be subdivided into a large number of reaction time steps. Additional computation effort is also required to reduce the splitting error. In this presentation, we develop exact solutions of various first-order reaction chains for the reaction operator and couple those solutions with numerical solutions of the transport operator. The reactions are treated as local phenomena and simulated using exact solutions that we develop, while the multiphase transport are treated as global processes and simulated numerically. The focus of this study is to develop analytical solutions of those radionuclide decay chains in the inventory and to implement the method in a multiphase transport code. The previous version of the NUFT code is a purely numerical suite for modeling multiphase, multicomponent reactive transport under non-isothermal conditions. It simulates multiphase advection, dispersion, reactions (both kinetics and equilibria), thermal conduction, and radiation, etc. in multiple overlapped porous and non-porous media. It has been successfully used in modeling of reactive transport with equilibrium reactions and non-stiff kinetic reactions. In this study, we develop a library of analytical solutions for all possible reaction chains, including stiff reactions, in the inventory. Then, the library directly supports NUFT simulations with single-step analytical solutions for all species. It is demonstrated that the incorporation of exact solutions for the reaction operator can eliminate the error from ODE solvers and significantly increase simulation speed. The new operator-splitting approach has been validated by comparison against an exact solution and a conventional operator-splitting solution. The approach offers both simulation accuracy and computational efficiency for modeling of radionuclide transport at Rainier Mesa compared to conventional OS methods.

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Semi-analytical solution of delineation of capture zone

Authors: Babak Shafei, Behzad Ataie Ashtiani

Pump-and-treat is one of the most widely used ground water remediation technologies and analysis of capture zone of pumping wells is a useful tool for designing these systems and well head protection programs. Semi-analytical solutions have been developed for defining the geometry of the capture zone for two different scenarios. In the first case a partially penetrating well with infinitesimal radius under a constant pumping rate in a two-zone confined aquifer is presented. Effect of well bore skin of finite thickness which is developed due to the process of drilling and stalling, will be considered and a sensitivity analysis is performed to study its effect on the location of the stagnation point, maximum horizontal and vertical extent of capture surface. The equations of streamlines are solved using the numerical procedure of Runge-Kutta. It is concluded that skin effect can be neglected when degree of the penetration of the well and well pumping discharge are increased. In practice where thickness of skin zone is less than the assumed values, its effect isn't a significant factor and geometry of capture surface can be obtained by assuming a single-zone aquifer. Effect of different parameters such as pumping rate, degree of penetration of well and thickness of skin zone are presented. In the second case a non-steady state analyses of the capture zone will be presented which is important in well head protection programs or pump and treat systems where the remediation process is done in a limited period of the time. A new transient semi-analytical solution is developed by applying the Laplace transform to combined discharge potential expression and substituting the related analytical Laplace domain solution of hydraulic head. The governing equations of the stagnation point coordinates and the differential equations of the streamlines are obtained in Laplace domain as well. Applying different existed hydraulic head solutions for different boundary conditions makes this solution flexible to be used to obtain the geometry of the capture zone in three dimensions for wide range of the remediation scenarios. The solution is applied to the case of partially penetrating well in a confined aquifer pumping under constant discharge. Time-dependent location of the stagnation point, maximum horizontal and vertical extent of the capture surface is presented applying different numerical methods such as forth order Runge-Kutta scheme and Stehfest Laplace inversion method. The transient characteristics of the capture zone are compared with the results of steady state solutions at late times.

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Separating 'Guts' and 'Garbage' in Earth System Models

Authors: Balazs M. Fekete, Charles J. Vorosmarty

Developing earth system models that can effectively utilize modern data management, distributed CPU computational resources and advanced visualization are becoming increasingly complex tasks. Earth scientists urgently require new modeling platforms to separate the science code (\"guts\" for an earth scientist) from the service infrastructure (\"garbage\" for the scientist). Numerous efforts are underway to simplify various elements of earth science applications, such as data access and management (OGC map and data services, OpeNDAP, standard data formats such as NetCDF, HDF, etc.) and basic modeling infrastructure (FMS from GFDL or ESMF from NCAR, OpenMI, etc.). The adaptation of these systems are still beyond the computer skills of most earth/hydrological scientists. The Water System Analysis Group of the University of New Hampshire has developed several modeling frameworks in the past decade that made in- house model development significantly easier and demonstrated the enabling power of a model development infrastructure, in this case dedicated to land surface hydrology simulation, river network analysis, and biogeochemical flux modeling. The core science components of Earth System models can be divided into two parts: the overall model structure and the actual implementation of individual physical or biogeochemical processes surrounded by support infrastructure that executes common tasks such as spatial and temporal domain management, model input/output, etc. This structural divide is captured well by the design schema of the Earth System Modeling Framework (ESMF) that provides standard interfaces to couple modules (as a model \"super-structure\") and support services to make the implementation of the individual modules easier. While ESMF and similar modeling frameworks provide significant code infrastructure for model development, their adaptation still has a steep learning curve. Developers need to understand concepts like domain decomposition, array communications (to make applications run on parallel computing platforms), module coupling, time management, etc. We argue that most of these components can be hidden from an intelligent user, and intelligent software designs could instead unburden the use by handling the coupling of different domains (such as atmosphere-to-land surface, groundwater to land-surface model, or land-surface to river network) or advancing time as needed by the individual modules. The ultimate aim is to structure such systems in such a way so as to enable scientists to focus on single module elements, their mathematical formulation, and the rules by which the modules interact with each other. In our presentation, we will demonstrate how our most recent modeling infrastructure - the Framework for Aquatic Modeling of the Earth System (FrAMES) - works, including its main design elements and implementation. We will discuss the strength and weaknesses of FrAMES, and outline the basic principles of a new modeling infrastructure. We recognize that developing a truly comprehensive modeling environment is beyond what a small research team can realize, so we would like to convince the scientific community that our vision is feasible as a consortium-based effort. We encourage collaboration to realize its full potential.

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Simulating historical changes in the hydrologic system of California's Central Valley with the California Central Valley Groundwater-Surface Water Simulation Model (C2VSIM)

Authors: Charles F. Brush, Emin C. Dogrul, Tariq N. Kadir, Michael R. Moncrief, Steve Shultz, Matt Tonkin, Daniel Wendell, Francis Chung

The California Central Valley Groundwater-Surface Water Simulation Model (C2VSIM) is an integrated hydrologic model developed using the Integrated Water Flow Model (IWFM) program. C2VSIM simulates land-surface, groundwater and surface-water flow in the alluvial portion of California's Central Valley, an area of approximately 52,000 km2 (20,000 mi2), with a monthly time step from October 1921 through September 2003. The Central Valley's hydrologic system experienced significant changes during this period as a result of steady agricultural expansion, extensive groundwater pumping, the development of surface water storage and conveyance systems, and recent urban expansion. A calibrated model will allow better understanding of historical water budget components, especially rates and distribution of groundwater pumping, and will serve as a useful planning tool to assess the impacts of regional water management programs such as conjunctive use of groundwater and surface water, changes in surface water inflows to the valley, or significant changes in land use. IWFM incorporates a three-dimensional finite element groundwater flow process dynamically coupled with one-dimensional land surface, river, lake and unsaturated zone processes and a simplified land-surface process to simulate surface and subsurface flows from ungaged small-stream watersheds adjacent to the model boundary. The groundwater flow system is represented with three layers of 1392 elements, the surface-water network is simulated using 433 river nodes representing 74 river reaches, with a single outflow point at the Carquinez Straits, and the small-stream watershed process calculates flows for 210 ungaged watersheds. Monthly input data include the elemental distribution of agricultural crops, urban area and native vegetation, precipitation, and evapotranspiration; boundary surface-water inflow at 40 gaged river locations; and 107 surface-water diversions from 97 diversion locations. The IWFM land-surface process partitions precipitation to infiltration and runoff, calculates aggregate water demands, routes runoff to rivers and deep percolation to the unsaturated zone, allocates available surface water to meet agricultural and urban demands, and calculates the amount of groundwater pumping required to meet the remaining demands (especially useful in California where groundwater pumping is not recorded), and the IWFM surface water process routes river flows and calculates stream-groundwater interactions. Optimum regional hydraulic parameters were calibrated using the parameter estimation program PEST and observations of groundwater head (H), vertical groundwater head gradient (V), groundwater-surface water interaction (I) and river flow (Q) for the period October 1975 through September 1999. Composite scaled sensitivities calculated for each parameter type and observation type demonstrate how the linkage of multiple hydrologic processes within IWFM facilitated model calibration. Saturated and unsaturated groundwater process parameters were extremely sensitive to V; river, lake and land-surface parameters were most sensitive to I followed by V; and small-stream watershed parameters were most sensitive to I followed by Q. Simulation results provide insight into the evolution of the groundwater flow system over time. Estimated groundwater extraction increased from approximately 5 km3/yr (6 million acre-feet [MAF]/yr) in the 1920's to a maximum of 19 km3/yr (16 MAF/yr) in 1977, and more recently declined to an average of 11 km3/yr (9 MAF/yr) between 1994 and 2003. Simulated groundwater discharges to rivers dropped from 3.6 km3/yr (2.9 MAF/yr) in the 1920's to 1.5 km3/yr (1.2 MAF/yr) between 1994 and 2003 as groundwater extraction altered groundwater flow patterns. Simulated evapotranspiration increased from 21 km3/yr (17 MAF/yr) in the 1920's to 34 km3/yr (28 MAF/yr) between 1994 and 2003 as agricultural and urban expansion supplanted native vegetation.

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Simulating Isolated Bacterial Microhabitats in Unsaturated Soil

Authors: Jessica Furrer Chau, Amvrossios C. Bagtzoglou, Dani Or

Bacterial diversity in soil exceeds by orders of magnitude that found in oceans and others compartments of the biosphere. There is strong evidence to suggest that spatial isolation imparted by fragmented aquatic microhabitats in unsaturated soil plays a large part in creating this diversity. This study aims to elucidate the role of soil texture, which determines the extent and connectivity of microhabitats, in constraining bacterial diversity. A range of soil samples of varying textures (sandy, silty, and clayey) was collected from sixteen locations across Connecticut and Massachusetts. Soil particle size distributions (PSD) were measured to obtain soil texture (determined by % sand, silt and clay) and for use in modeling. A 3-D model of each soil sample was constructed using the measured PSD, and a lattice Boltzmann model was used to simulate the location of isolated water pockets which could serve as bacterial microhabitats. In this way an estimate was obtained of the maximal diversity that could be sustained in the soil. Molecular analysis (T-RFLP technique) was performed to evaluate the diversity of the bacterial communities in the samples for comparison with the modeled values. We present the results of this comparison and discuss the findings in terms of relevant soil physics considerations. Microbially-mediated biogeochemical processes occur at and below the pore scale, but we measure them at the bulk scale. Pore scale fluid modeling with the lattice Boltzmann method is a tool that can connect the two scales; predicting diversity using pore-scale fluid modeling shows that we understand spatial distribution of bacteria at the pore scale. This information could then be applied to problems such as transport in the vadose zone.

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Simulating Runoff from a Grid Based Mercury Model: Flow Comparisons

Authors: Heather E. Golden, Christopher D. Knightes, Robert B. Ambrose, Jr.

Several mercury cycling models, including general mass balance approaches, mixed-batch reactors in streams or lakes, or regional process-based models, exist to assess the ecological exposure risks associated with anthropogenically increased atmospheric mercury (Hg) deposition, soil Hg concentrations, and consequent surface water fluxes. However, few mercury models exist at the scale of watersheds and include the coupling of processes involving multiple sources (atmospheric and terrestrial) and transformations of Hg, and watershed loading to surface water bodies. This is particularly important in large basins, where few mercury modeling studies have been conducted. We are refining a grid-based watershed Hg model (GBMM v2.0, Tetra Tech, 2006) that computes mass balances for hydrology, sediment, and mercury within each GIS raster grid cell and produces flux estimates of each to a tributary network. Daily runoff is a critical process governing surface water contaminant concentrations and volumetric flow rates in GBMM; thus, assessing whether we best capture observed runoff using a grid-based curve number approach compared to other established models is an important exercise. We compare the daily runoff generation from GBMM to a semi-distributed nutrient fate and transport model and a semi-distributed hydrological model to evaluate the hydrological component of this pilot model. Further, we explore the structural differences of the water balance and runoff generation mechanisms in the models to evaluate which approach best fits the objectives of GBMM to predict mercury concentrations in rivers and streams. Preliminary results suggest that the grid-based curve number approach to runoff generation represents flows relatively well during years without extreme weather events (i.e., droughts or flooding) but may distort runoff predictions in coastal plain settings. Disclaimer: Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

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Simulation and Management of Regional Scale Groundwater Flow Systems

Authors: Kenneth Belitz, U.S. Geological Survey, California Water Science Center and Randall Hanson, U.S. Geological Survey, California Water Science Center

By definition, regional groundwater flow systems are large. Therefore, modelers face the challenge of resolution. This challenge is not limited to selection of the appropriate spatial and temporal scales for modeling; it also includes issues related to data synthesis, data assimilation, and coupling of the groundwater flow system to other components of the hydrologic cycle. These issues can become significant obstacles to evaluation of regional scale management solutions.

This session will focus on contributions that advance our ability to represent, simulate, or manage regional groundwater flow systems. Examples include representation of regional scale subsurface heterogeneity; incorporation of natural and engineered surface-water networks into groundwater models; harnessing of real-time and near real-time datasets for model input and model calibration; incorporation of water quality monitoring networks into groundwater models; coupling of regional scale groundwater models with models representing other processes; coupling of models at different scales; and incorporation of decision making into regional groundwater models. Contributions at the interface between new methods and their application to important aquifer systems are especially encouraged

Simulation of 14C Dispersal by CO2 Gas Bubble Expansion from Nuclear Test Detonation in Unsaturated Carbonate Rock

Authors: Steven F. Carle, Mavrik Zavarin, Yunwei Sun, Gayle A. Pawloski

659 underground nuclear tests were conducted in tunnels, shafts, and craters in Yucca Flat at the Nevada Test Site (NTS), Nevada. Most underground nuclear tests were conducted above the water table in siliceous alluvial or volcanic rocks with water contents ranging from 5-20%. However, four tests were situated in carbonate rock of relatively low water content (<1%). These carbonate tests released voluminous quantities of CO2 by thermally decomposing dolomite or limestone. If CO2 gas flow processes are excluded, radionuclide transport models suggest radioactive carbon-14 (14C, half-life 5,730 years) can dictate the outer spatial extent of the 4-millirem regulatory limits on radioactive dosage defining groundwater contamination by underground nuclear testing at NTS. However, carbonate tests are unique in that CO2 is the dominant gas produced immediately after detonation, rather than water vapor. Radioactive 14C is partitioned into this test-released CO2, which also redistributes other volatile radionuclides such as tritium and 85Kr. Differences in pressure and temperature dependent phase equilibrium relationships cause differences in the spatial distribution of 14C, tritium, and 85Kr over time. This study uses numerical simulation of thermal multi-component coupled gas-liquid phase flow and transport to investigate how CO2 gas release affects transport of 14C and other radionuclides over distances of hundreds of meters. Simulations are calibrated to post-test data from the Handcar and Nash carbonate tests detonated in 98% dolomite hundreds of meters below the ground surface. The Handcar test released about 1,800 metric tons of CO2 based on post-test gas sampling. Gaseous radionuclide transport was confirmed within weeks after detonation by radioactivity detected 94-120 meters from the Handcar detonation location. Measured gas composition of 2/3 CO2 and 1/3 air in a cavernous post-test collapse-induced void located 50-68 m above the detonation location indicates test-released CO2 lingers in the vadose zone for years after detonation. Numerical simulations suggest the Handcar data can be explained by initial rapid expansion of a high pressure and temperature CO2 gas bubble followed by downward density flow, gaseous diffusion, and partitioning to liquid phase. Our simulations predict test-derived 14C and other volatile radionuclide gases would reach the water table 200 m below in a timeframe of several years to decades. The Nash test was detonated closer to the water table compared to Handcar. Water level data, pumping history, and concentrations of tritium, 14C and other volatile radionuclides are available from a well installed 10 years after the Nash detonation 183 meters downgradient. Numerical simulations suggest most of the tritium was flushed into the saturated zone by drainage of water out of collapsed rubble above the Nash test. The 14C/tritium ratio measured in the downgradient well near Nash indicates depletion of 14C, consistent with simulation results showing dispersal of 14C by the CO2 gas bubble expansion. Our thermal multi-phase flow and transport simulations indicate CO2 gas bubble expansion disperses 14C and other volatile radionuclides into the vadose zone. CO2 gas expansion could also enhance dispersal of 14C away from unsaturated tests detonated in carbonate-rich alluvium. Addition of test-released CO2 flow processes to 14C transport modeling can substantially reduce the contribution of 14C to predicted extent of groundwater contamination from radionuclide release by underground nuclear testing at NTS. LLNL-ABS-400484. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract No. DE-AC52-07NA27344. This work was performed in support of the National Nuclear Security Administration, Department of Energy, Nevada Site Office, Underground Test Area Project.

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Simulation of 3H-3He Groundwater Age by Coupling Gas and Liquid Phase Transport Processes from the Surface to the Saturated Zone

Authors: Steven F. Carle, Jean E. Moran, Brad K. Esser

Groundwater age estimates determined from environmental tracers are extremely useful for calibration of groundwater flow and transport models because potentiometric data and pumping rates alone are usually not sufficient to calibrate model fluxes, particularly recharge rates. However, difficulties arise in the use of age data in models because of complexities of surface, vadose zone, and groundwater flow processes affecting transport of tracer constituents, including (1) transients in isotopic source concentrations, pumping rates, and water table elevation, (2) mixing caused by long well screens, dispersion, and heterogeneity, and (3) isotopic constituent property differences in molecular diffusivity and solubility. Tritium (3H), a radioactive isotope of hydrogen, decays to helium-3 (3He) with a half-life of 12.3 years. The 3He/3H ratio in water can be used to estimate groundwater age to within one year or less over a 50 year timescale. Tritium in precipitation from cosmogenic and anthropogenic (bomb pulse) sources percolates through the vadose zone and into groundwater as HTO. 3He has a very low solubility in water and remains mostly in the gas phase in unsaturated conditions. In the saturated zone, 3He dissolves into the liquid phase at concentrations well below solubility limits. Tritiogenic 3He concentrations in water increase below the water table with radioactive decay of 3H. Assuming non-reactive tracer transport of 3H and 3He below the water table, 17.8 ln[1+3He/3H] yields the “apparent age” as years of water molecule travel time in saturated conditions since reaching the water table. We use a coupled liquid-gas phase variably saturated groundwater flow and transport model to link 3H and 3He transport with surface, vadose zone, and groundwater flow processes in a 3 km X 3 km area of a shallow water table aquifer in the southern San Joaquin Valley, California. The model is centered on a dairy farm where feed crops are intensively irrigated with shallow groundwater, resulting in seasonal irrigation return through the vadose zone. Regionally, the water table varies from pumping and irrigation with ground and surface water. Subsurface heterogeneity is modeled using a transition probability-based geostatistical model of fluvial architecture of sandy channels embedded with silt and clay lenses calibrated to 11 continuous CPT profiles. 3He/3H age data were obtained at several irrigation and multi-level monitoring wells. In the model, the ground surface is used as a boundary condition for recharge fluxes, liquid phase concentrations of 3H (from measurements in precipitation and surface water), and gas phase concentrations of 3He (from atmospheric conditions). Gas-liquid phase equilibrium for 3H and 3He is constrained by established temperature and pressure-dependent solubility relationships. Thus, coupling of gas-liquid phase flow and transport assuming equilibrium gas-liquid partitioning governs simulated transport of 3H and 3He and subsequent simulation of apparent groundwater age. In this study, 3He/3H groundwater age is simulated by coupling gas-liquid 3H and 3He transport processes between the ground surface, vadose zone, saturated zone, and pumping and monitoring well intakes. Typical groundwater flow models only compare advective flow paths to isotopic age estimates without addressing important complexities, particularly mixing at wells, heterogeneity, transients in isotope surface concentration, gas-phase partitioning, vadose zone processes, and water table fluctuations. The coupled gas-liquid phase simulation framework presented here enables comparison of apparent 3He/3H age with true age in a realistic setting. In general, simulated apparent ages are within 10% of true ages for the conceptual model studied. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract No. DE-AC52-07NA27344.

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SIMULATION OF CONJUNCTIVE USE IN REGIONAL AQUIFER SYSTEMS USING MODFLOW's FARM PROCESS

Authors: HANSON, Randall T.[1], SCHMID, Wolfgang[2], FAUNT, Claudia C.[1] , and Belitz, Kenneth[1]
[1] U.S. Geological Survey, 4165 Spruance Rd, Suite 200, San Diego, California, 92101-0812, (619) 255-6139/-6142, E-mail: rthanson@usgs.gov/ccfaunt@usgs.gov/kbelitz@usgs.gov
[2] Department of Hydrology and Water Resources, University of Arizona, P.O. Box 210158-B, Tucson, AZ 85721-0158, (520) 621-1083, E-mail: w_schmid@hwr.arizona.edu

The new Farm Process (FMP) allows simulation of land-use processes affecting the movement and use of surface and ground water with the U.S. Geological Survey's hydrologic model, MODFLOW (MF2K). The MF2K-FMP is used to assess water availability for developed and undeveloped land use. Because FMP is fully coupled with simulations of ground-water and surface-water flow, it can be used as a tool to investigate linkages between management decisions and the availability of water. The FMP was applied at scales ranging from the 20,000-square-mile (mi^2) Central Valley of California to the 160-mi^2 Pajaro Valley, a coastal watershed of Monterey Bay. The FMP integrates simulation of water supply and demand, which facilitates the simulation of water movement in complex and heavily developed water-resource systems. The FMP is especially useful in settings where historical ground-water pumpage is unknown, or where estimates of future pumpage on the basis of anticipated natural or anthropogenic demands are needed.

The Central Valley and Pajaro Valley are two very productive agricultural regions in California. Expansion of irrigated agriculture and growth of urban population has increased the competition for surface and ground water. The MF2K-FMP was used to simulate the conjunctive use of surface and ground water in these two valleys. The FMP was used to estimate historical pumpage and delivery of surface water (1960s to present) for 21 water-balance subregions in the Central Valley and 24 subregions in Pajaro Valley. The simulations indicate that surface-water delivery provides most of the agricultural demand early in the growing season in the Central Valley, augmented with ground-water pumpage later in the season. The relative proportions of surface water and ground water used for irrigation in the Central Valley also vary from year to year in response to climate and import availability. In contrast, the ground water used for irrigation in the Pajaro Valley is significantly augmented by precipitation early in the growing season. These models are being used to evaluate the effects of conjunctive use. The application of the Farm Process and MODFLOW facilitates the analysis of the effects of development on the supply and demand components of surface water and ground water.

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Simulation of enhanced dynamic Interaction between Surface and Groundwater in a conjunctive Use Area

Authors: W. Bejranonda, S. Koontanakulvong, M. Koch

Rice cultivation is the dominant agricultural activity in Thailand. Not only has rice historically have had a particularly esteemed standing in Thai culture, is has become nowadays also a major cash crop for the Thai economy as a whole. However, rice growth is intricately dependent on huge amounts of irrigation water. As the latter is being drafted increasingly from groundwater resources, this has put pressure not only on regional aquifers, but owing to river-groundwater interactions, also on surface water resources which in turn are also the major water source for many Thai urban areas. As part of a major national effort, conjunctive water uses are to be explored to optimize the water resources for the various stakeholders involved. Providing irrigation water through irrigation canals sipping adjacent streams has been the classical approach method in so-called irrigation projects in Thailand to augment the agriculturally available water there during a dry season or drought periods, the latter becoming more frequent in recent years. As the canal irrigation water has to be increasingly complemented by pumped groundwater, complex surface-groundwater interactions occur which need to be understood for the setup of a comprehensive water balance analysis. This is the objective of the present conjunctive use study wherein a newly developed semi-coupled surface- groundwater model will be employed. Surface and groundwater dynamic interactions in the Upper Great Chaophraya Plain of Thailand are being explored. The study area is mainly composed of 5 river basins. In the study area, 63% of the basin is dedicated for agricultural activities that are relying on conjunctive water use. The surface-soil water model SWAT and the groundwater model MODFLOW are semi-coupled to determine the hydrological components and their effects on flow behaviour and. For the SWAT surface water model the 5 main stream basins are divided into 22 sub-basins, while the MODFLOW subsurface model is built up with 2 layers and 666 grid-cells. Interactions between surface-water and groundwater through the surface recharge and the river-aquifer interactions are used to couple the models. When the combined model is operated under the “coupling process”-mode, SWAT and MODFLOW are connected through some selected components that are expressed in form of duplicated functions. An interface program has been developed to transmit model information directly to the coupling process. The coupled models are executed by running simulations individually while monthly river-groundwater interaction and groundwater recharge are employed to generate the surface-groundwater dynamic interaction functions. Calibration results for observed hydrographic time series in the time-interval 1993-2003 indicate that the coupled model significantly improves both streamflow and groundwater simulation, namely, the water balance analysis. Furthermore, streamflow and groundwater level calculations, especially in the dry season, are improved by 12% and 2.3%, respectively. The interaction is season-dependent, i.e., the rivers recharge 0.8 mm. of rainfall into the aquifers during the wet season while the aquifers provide baseflow of 10.4 mm. to the rivers in the dry season. This shows that streamflow is an important source of groundwater recharge and helps to maintain the groundwater levels beneath the agricultural area, so that farmers are able to pump groundwater from their own wells. Groundwater wells can thus serve as a secondary source of irrigation water, relieving farmers of imminent water shortage.

Simulation of enhanced dynamic interaction between surface and groundwater in a conjunctive-use area with a semi-coupled model

Authors: Werapol Bejranonda, Sucharit Koontanakulvong, Manfred Koch

Rice cultivation is the dominant agricultural activity in Thailand. Not only has rice historically have had a particularly esteemed standing in Thai culture, is has become nowadays also a major cash crop for the Thai economy as a whole. However, rice growth is intricately dependent on huge amounts of irrigation water. As the latter is being drafted increasingly from groundwater resources, this has put pressure not only on regional aquifers, but owing to river-groundwater interactions, also on surface water resources which in turn are the major water source for urban areas. Mathematical models are important tools in water resources planning and management. Surface water and groundwater models have been used to estimate water budgets available for management and allocation but, for expediency, these have been employed mostly in a decoupled manner or, slightly better, using only one-way forward approach at the surface- groundwater model boundary. When groundwater use was hugely rising and hydrological elements of whole water system are needed to fully manage, the coupling simulation of both surface and subsurface simulation was then developed clarifying the water balance. Surface and groundwater dynamic interactions in the Upper Great Chaophraya Plain of Thailand are is being explored. The study area is mainly composed of 5 river-basins. In the study area, 63% of the basin is dedicated for agricultural activities that are relying on conjunctive water use. The surface-soil water model SWAT and the groundwater model MODFLOW are semi-coupled to determine the hydrological components and their effects on flow behaviour and. For the SWAT surface water model the 5 main stream basins are divided into 22 sub-basins, while the MODFLOW subsurface model is built up with 2 layers and 666 grid-cells. Interactions between surface-water and groundwater through the surface recharge and the river-aquifer interactions are used to couple the models. When the combined model is operated under the “coupling process”-mode, SWAT and MODFLOW are connected through some selected components that are expressed in form of duplicated functions. An interface program has been developed to transmit model information directly to the coupling process. The coupled models are executed by running simulations individually while monthly river-groundwater interaction and groundwater recharge are employed to generate the surface-groundwater dynamic interaction functions. Calibration results for observed hydrographic time series in the time-interval 1993-2003 indicate that the coupled model significantly improves both streamflow and groundwater simulation, namely, the water balance analysis. Furthermore, streamflow and groundwater level calculations, especially in the dry season, are improved by 12% and 2.3%, respectively. The interaction is season-dependent, i.e., the rivers recharge 0.8 mm. of rainfall into the aquifers during the wet season while the aquifers provide baseflow of 10.4 mm. to the rivers in the dry season. This shows that streamflow is an important source of groundwater recharge and helps to maintain the groundwater levels beneath the agricultural area, so that farmers are able to pump groundwater from their own wells. Groundwater wells can thus serve as a secondary source of irrigation water, relieving farmers from water shortage. The Plaichumpol Irrigation Project, a pilot area located between 2 main rivers in the Great Chao Prhaya Plain, was selected to explore in more detail the surface- groundwater interactions as a function of rainfall, irrigation supply and groundwater extraction during the course of years comprising both a wet and dry season. Additionally, the administered irrigation plan and the surface water conditions were used to set up a pumping scheme in the groundwater model. The coupled-model simulations showed that, for sustainable water allocation in the irrigation area, a conjunctive use of surface- and groundwater is required.

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Simulation of Subsurface Biological Systems using Cellular Automata

Authors: Ganesh Oka, George F. Pinder

Simulation of Subsurface Biological Systems using Cellular Automata Ganesh Oka and George F. Pinder College of Engineering and Mathematical Sciences University of Vermont Burlington, Vermont The growth in bacterial biomass brings about a change in hydraulic conductivity of the host soil which, in turn, changes the distribution pattern of the contaminant as it undergoes biodegradation. The modeling of growing biomass can be studied using cellular automata (CA) at the pore level. On the other hand, the modeling of contaminant distribution is based on balance equations formulated at the porous medium scale obtained by averaging the extensive quantities, like mass and momentum, at the pore level,. The momentum balance equation at the porous medium scale involves terms describing the resistance offered to the flow of water as it passes through the porous medium. The CA is specifically designed to calculate the resistance offered by solid surface-biomass combination. Thus it is possible for the CA to provides an input at the microscopic level to be used to define terms in the macroscale momentum balance equation that describe the resistance offered to the flow of water; thus changing the hydraulic conductivity of the soil. The resulting equations provide the mathematical foundation upon which a biodegradation simulation model is constructed. Computed results show the feasibility of this approach to biodegradation simulation.

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Simulation of Turbulent Sedimentation in Flocculent-Aided, Storm-Water Retention Basins: Formulation and Computational Challenges

Authors: Joon Lee, Fred Molz, Abdul Khan, Mark Schlautman, Dennis Stevenson

Particle flocculation, fragmentation, settling and possibly lithification in a turbulent flow-field underlies many problems in water resources and sedimentary geology. This problem must be studied within a particular context , but the overall topic is found in many areas of engineering and science. The most rigorous formulation of turbulent sedimentation involves solving the Navier-Stokes equations along with the full population balance equations. While less detailed formulations have been studied on large scales, such as river basins, our formulation has been studied rigorously to date only on small laboratory scales. Sediment deposition in geologic systems often involves turbulent sedimentation in a variety of environments, and the nature of natural heterogeneity is still not well understood. So the research to be presented has potential applications in many areas of sedimentary geology. In the water resources area, particle flocculation and sedimentation is central to many water treatment and waste treatment processes, to water quality in rivers, lakes and estuaries and to air quality. Many of the most recent fundamental studies of turbulent sedimentation are found in the chemical engineering literature. In its most general form, the required mathematics and computational demands are extensive, and only recently has it become practical to simulate the overall process using computational approaches that are becoming readily available. Herein we describe applications of the population balance equations coupled to the Navier-Stokes equations to simulate turbulent sedimentation in flocculent-aided retention basins. The operation of such ponds is complicated, involving turbulent flow of variable intensity, different pond geometries, particle growth due to flocculation, fragmentation of larger particles, and settlement of particle size classes at different rates. Currently, we are solving the N-S equations for steady-state conditions using commercial software called FLOW3D. Code for solving the discrete population balance (DPB) equations has been developed “in house”, and it is based on the binary model for the particle classes and the aggregation and breakage terms. Such a model can cover the range of possible particle sizes using 30 coupled PDEs. Two-D versions may be solved on a modern PC (8 hour run times), but three-D solutions rely on the use of high throughput computing, as opposed to high performance computing. High throughput computing is applicable when a large number of independent runs must be executed over and over, such as the series of iterations needed to solve a collection of sets of nonlinear algebraic equations (one system matrix for each individual DPB equation). We have so-called middleware (CONDOR) that enables one to run standard programs on un-utilized personal computers, such as those in student computer labs in the late evening and early morning hours. CONDOR manages efficiently a cluster (10s 100s, etc.) of machines, as well as handling other computational resources such as server and disc farms. Unlike high performance computing, which generally requires reprogramming legacy codes, high throughput computing can run legacy codes (FORTRAN, C++, etc.) with essentially no changes. Flocculation and sedimentation processes in an idealized storm-water retention basin are simulated by first solving steady-state versions of the Reynolds-averaged Navier Stokes (RANS) equations. Output from the RANS equations is input to the 30 nonlinear PDEs constituting the DPB equations, which essentially are coupled reactive transport (advective-diffusion) equations with source and sink terms. Run times are greatly reduced with the aid of CONDOR.

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Soil-Root Interactions Controlling Plutonium Transport in Variably Saturated Soils

Authors: Inci Demirkanli, Fred Molz, Dan Kaplan, Robert Fjeld

To better understand longer-term vadose zone transport in southeastern soils, field lysimeter experiments were conducted at the Savannah River Site (SRS) near Aiken, SC, in the 1980s. Each of the three lysimeters analyzed herein contained a filter paper spiked with different Pu solutions, and they were left exposed to natural environmental conditions (including the growth of annual weed grasses) for 11 years. The resulting Pu activity measurements from each lysimeter core showed anomalous activity distributions below the source, with significant migration of Pu above the source. Such results are not explainable by adsorption phenomena alone. A transient variably saturated flow model with root water uptake was developed and coupled to a soil reactive transport model. Somewhat surprisingly, the fully transient analysis showed results nearly identical to those of a much simpler steady flow analysis performed previously. However, all phenomena studied were unable to produce the upward Pu transport observed in the data. This result suggests another transport mechanism such as Pu uptake by roots and upward transport due to transpiration. Thus the main objective of the present talk is to describe the extension of the variably saturated flow and reactive transport model to include uptake and transport of Pu within the root xylem, along with computational methodology and results. The five equations comprising the transient flow model and the transport models for Pu migration in the soil and plant will not be listed here due to space limitations. Using a finite-difference approach, the overall problem involves the coupled solution of one flow equation (Richards Equation with a root water uptake sink term) and four transport equations (two in the soil and two in the root xylem). Flow velocity in the soil was driven by precipitation input along with transpiration and drainage output. The calculated velocity distribution drove the advection and dispersion of the 2 (reactive) Pu species in the soil. Water uptake by the roots due to transpiration determined the flow velocity in the root xylem, and this along with uptake of Pu in the transpiration stream drove advection and dispersion of the two Pu species (to date non-reactive) in the xylem. A numerical problem that resulted was due to the large mismatch of flow velocities in the soil and plant xylem. During wet periods with high potential evapotranspiration, it was estimated that maximum flow velocities through the xylem would approach 600 cm/hr. This is many orders of magnitude larger that flow velocities in the soil, resulting in very different Peclet numbers. With the inclusion of Pu uptake by grass roots and translocation in the transpiration stream, it is easy and natural to simulate both the upward and downward movement of Pu activity that was observed in the experiments. This leads to the following tentative conclusions: 1) Hysteresis, extreme root distribution functions, air-content dependent oxidation rate constants, and large evaporation rates from the soil surface were not able to explain the observed upward migration of Pu. 2) Small amounts of Pu uptake by plant roots and translocation in the transpiration stream creates a realistic mechanism for upward Pu migration, and is also consistent with the previously simulated downward movement in the soil. 3) Realistic xylem cross-sectional areas imply high flow velocities (hundreds of cm/hr) under hot, wet conditions. Such flow velocities produce the correct shape for the observed activity distributions in the top 20 cm of the lysimeter soil. 4) Simulations imply that Pu should have moved into the above-ground grass tissue each year during the duration of the experiments, resulting in an activity residual accumulating on the soil surface. Lysimeter data now being analyzed may support this prediction.

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Solid Phase Transformation And Biomass Accumulation During Uranium Bioremediation At Rifle, Colorado

Authors: Li Li, Carl I. Steefel, Kenneth H. williams, Mike Wilkins, Andreas L. Englert, Susan S. Hubbard

In situ uranium remediation involves the injection of chemicals as electron donors into the subsurface to stimulate indigenous bacteria that can transform the soluble U(VI) to insoluble U(IV), therefore immobilizing uranium. Such perturbation often leads to complicated biogeochemical reactions coupled with transport processes, as well as changes in solid phase composition and biomass accumulation, which can potentially alter the subsurface properties and therefore affect the remediation efficiency. Although aqueous geochemistry data are routinely collected during field scale remediation experiments, quantification of the evolution of solid phase and biomass remains challenging, partly due to the expense, time, and efforts involved. In this context, reactive transport modeling works as an efficient, cost-effective, and non-destructive tool to identify the dominant biogeochemical processes and to provide information about the solid phase transformation associated with field scale bioremediation processes. In this work, we combine reactive transport modeling with column experiments and field measurements to understand the biogeochemical reaction processes, and to quantify the biogeochemical reaction rates and the solid phase transformation associated with a field-scale uranium bioremediation experiment at Rifle, Colorado. The column experiment was carried out using the natural sediments collected from the Rifle site and under conditions similar to the field experiment. The reactive transport model CrunchFlow couples the biogeochemical, transport, and microbial processes. The rates of biogeochemical reactions are characterized by dual Monod rate laws with an inhibition term, which can simulate the redox sequence. The rate law also includes an explicit incorporation of the rate dependence on biomass. Column experiment and modeling results show that the injection of the organic substrate acetate leads to the stimulation of dissimilatory iron oxide reducers, which transform the soluble U(VI) to the insoluble U(IV). After the depletion of bioavailable iron oxide, sulfate reduction starts, although it does not facilitate the reduction of U(VI). The products of these biogeochemical reactions lead to the precipitation of secondary minerals, predominantly calcite and iron sulfide. Besides these main driving force of the system, the reaction network also includes adsorption of Fe(II) and uranyl to the surface of iron oxide occurs through surface complexation and instantaneous speciation reactions that occur in the aqueous phase. Using constraints provided by the 1D field aqueous data, modeling of the field-scale processes with the same set of reaction networks shows that the biogeochemical reactions proceed at their maximum rates close to the injection wells where the acetate concentration is highest. As a result, a maximum amount of calcite and iron sulfide precipitation and biomass accumulation occur at these locations, reaching as high as 2% of the pore space. The rates of the microbe-mediated reactions, including both iron oxide and sulfate reduction, vary significantly with time and space due to the spatial variation in acetate, iron oxide, and biomass concentration during the field experiment. Although the column experiments can be modeled using the dual Monod rate law without an explicit incorporation of the biomass term, such exercise for the field scale processes leads to an underestimation of rates close to the injection wells and an overestimation of rates far away from the injection wells. This may imply that the common exercise of using a rate law without a dependence on biomass can lead to errors in modeling field scale biogeochemical processes, where the amount of biomass varies significantly with time and space.

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Solute displacement by shock wave through saturated deformable porous medium: Characteristic and numerical solutions

Authors: Yuval Ohana, Shaul Sorek, Georgy Burda, Amit Gross

A one dimensional characteristic and numerical solutions address solute migration subsequent to an abrupt pressure change applied to a variable density Newtonian fluid, saturating a deformable porous medium (Sorek 1996). Mass and momentum balance equations for the fluid and an elastic matrix together with the solute mass balance equation, are solved by a general characteristic solution concerning the formulation of a traveling wave accounting also for the formation of shock waves, and by a numerical scheme implementing the Total Variation Diminishing (TVD) scheme. For a slightly deformable porous matrix the numerical simulation predicts the propagation of a single wave through the matrix at a sound speed of an apparent new fluid. In the case of a deformable matrix, this predicts the propagation of separate waves through the fluid and the matrix. Without Forchhaimer terms, properties (e.g. fluid velocity, fluid density, pressure, porosity and solute concentration) along the propagation route, retrieve their previous initial values after terminating the application of the abrupt pressure changes at the domain boundary. Accounting for Forchhaimer terms causes inertia exchange between the waves through the fluid and the matrix, and properties along the propagation route do not return to their initial stage.

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Some comments on upscaling.

Authors: Brian D Wood

We often think of upscaling as a process by which we develop macroscale equations for transport of mass, momentum, or energy with a reduced number of degrees of freedom. However, it is not the process of upscaling itself that leads to these simplifications, but rather assumptions (or 'scaling laws') imposed about the temporal-spatial structure of the phenomena of interest. Curiously, research employing upscaling methods is often mathematically fastidious in terms of the averaging process itself, but then imposes significant assumptions about the structure of the physical phenomena without significant fanfare. To illustrate this facet of the upscaling process, a fully nonlocal model describing macrodispersion in porous media is developed. Then, the influence of various assumptions about the structure of the Darcy-scale velocity vector and dispersion tensor fields is examined. This allow one to show that, although a fully nonlocal model can be considered to be a more exact representation of reality, this additional information comes with some cost. Nonlocal models also demand more information input, and thus require more effort to use both from the theoretical or applied perspective. In the most general case, the nonlocal model has the same information content as the original Darcy-scale representation. It is not until certain simplifying assumptions (scaling laws) are imposed that the nonlocal model shows a reduction in the number of degrees of freedom over that seen for the fully detailed Darcy-scale model. Implications will be discussed in the context of information content and the effective representation of complex systems with large numbers of degrees of freedom.

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Space-time optimization using a genetic algorithm within a sequential heuristic for groundwater quality sampling network

Authors: Roel Simuta, Graciela S. Herrera, J. Longina Castellanos

Long-term groundwater quality monitoring systems are an aid for groundwater contamination studies, but they represent the component of highest cost, because they include the costs associated with wells operation and sample analysis. For this reason an important problem is how to reduce the costs associated with groundwater quality monitoring without significantly reducing the quality of the estimation that can be obtained from the collected data. The subject that considers this problem is known as Sampling Networks Optimal Design. Such reduction can be obtained through the sampling of less wells, or sampling the same wells but with a reduced frequency of time, or by a combination of both strategies. A basic sampling network design principle is that an effective strategy should result in the selection of samples from wells such that they do not provide redundant information in space and time (spatial and temporal redundancy). The methodology for sampling network design used in this work is the same as that presented in Herrera and Pinder (2005). It is divided into three parts: (1) a flow and transport stochastic model is used to calculate an initial estimation of the concentrations of the contaminant in different positions and times, and their covariance matrix, by means of stochastic simulation, (2) a Kalman filter is applied to predict the uncertainty that the estimation of the concentration will have if the concentration obtained from samples taken in a set of positions in different times were used to update the initial estimation and (3) postprocessing, a procedure to produce a contaminant concentration estimate and to update it as data become available. A function of the estimation uncertainty is used as a criterion to choose the sampling wells and the sampling times for each well. In this work the total variance was used as a measure of the uncertainty level. Herrera and Pinder used a sequential method for optimizing the sampling network which chooses the space-time point that reduces the most the uncertainty in each step, and terminates when a predetermined value is reached. In this paper a genetic algorithm is used within a sequential heuristic method to obtain a smaller variance value,. At each step a new space-time position of a well is added, been either the one obtained for the Herrera and Pinder method or a random one, according to which gives the best function value. The method was tested with a synthetic problem. A contaminant source, located on the left-hand side of a 500 m by 700 m region, started to be active 24 years ago. Three years ago, three drinking wells were installed in the area extracting water at a 432 m3/d rate; these wells are still active. After an investigation it was found that the site is contaminated but the contaminant has not reached the drinking wells. It was decided to install a pump and treat system consisting on three injection wells and three extraction wells, all of them at pumping a rate of 1300 m3/d. A transient flow and transport model calibrated with the historical data is available for the site. It includes also a 2-year prediction period for the pump and treat system. The objective of the contaminant-sampling program is to estimate the contaminant concentrations at the three drinking water wells every 6 months during a 2-year period. After this period the sampling network and its sampling program is going to be reevaluated and updated with the generated data. A comparison of the optimization results when the two methods are applied to this example will be presented. References Herrera, Graciela and George Pinder, (2005): Space-time optimization of groundwater quality sampling networks, Water Resources Research, Vol. 41, W12407. doi:10.1029/2004WR003626.

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Spectral analysis of the ground water flow balance equation: implication for forward and inverse problems

Authors: Chiara Vassena, Mauro Giudici

The study of flow and transport phenomena in such heterogeneous systems as the porous geological formations can be described at very different scales. The fundamental equations are based on conservation principles and phenomenological physical laws, which relate the mass, energy or momentum fluxes to gradients of intensive quantities (potentials) that describe the state of the system under study. If ground water flow is taken as a reference test, the balance equation relates the piezometric head (h) with the hydraulic conductivity (K) field and the source/sink terms (F). This is: (1) a second order PDE for h which is the core of the forward problem to be solved to forecast the state of the physical system; (2) a first order PDE for K which is the core of the inverse problem to be solved for model calibration; (3) an explicit equation for F. Spectral analysis of the resulting balance equation permits to evaluate its filtering behavior. The joint use of Fourier analysis and asymptotic expansions permits to assess the spectral properties of the balance equation. In particular it is apparent that solving the forward problem (computing h from K and F) is equivalent to a filter that suppresses the components at high wave numbers. This property has important implications on the lack of stability of the inverse problem (computing K from h and F) and of the computation of F from measurements of h and K.

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Stability criteria for heterogeneous density driven flows

Authors: Sabine Attinger, Jude Musuuza, Florin Radu

Density-driven flows occur in deep aquifers due to temperature differences, in coastal aquifers due to salt mass differences but also in contaminant migration at refuse dumps. Its relevance cuts therefore across many applications like exploitation of geothermal energy resources, oil recoverly from aquifers and remediation of contaminated sites. A typical feature of density dependent flow problems is that they can become unstable (physically or numerically). A big challenge todate is to derive a general criterion that states the following two properties of the flow problem: 1. Is the flow physically stable or unstable? and 2. What is the computational grid resolution one needs to solve problem without creating numerical (artificial) instabilities? Here, we present new explicit criteria based on techniques from homogenization and perturbation theories. The work continues the ideas developed in [1]. The criteria include the effects of density and viscosity differences as well as subsurface heterogeneities. The validity of the criteria is carefully tested in numerical simulations varying dispersivities, mesh diameter, time step, etc over a large parameter range. The numerical simulations are performed with the software toolbox UG. [1] Held, R., S. Attinger, and W. Kinzelbach (2005), Homogenization and effective parameters for the Henry problem in heterogeneous formations, Water Resour. Res., 41, W11420, doi:10.1029/2004WR003674.

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Steady-state analysis of Effect of Proposed Dredge Material Containment Facility upon Freshwater Aquifers

Authors: Mark Cowan, Dr. Fred Tracy, Earl Edris, Dr. Jerry Lin, David Richards, Dr. Robert Wallace

The purpose of this research was to determine if a proposed saltwater dredge material containment facility would adversely affect nearby freshwater aquifers. The USACE District Office provided the researchers with (1) a high-resolution overhead (airplane) photograph of the study area, (2) LIDAR data of the study area, and (3) commercially contracted borehole drilling information. The researchers registered the LIDAR data with an overflight photograph using commercial off-the-shelf (COTS) software. The Groundwater Modeling System software (GMS version 6.0) was used to demarcate the area of interest, especially to cut away distant, obviously unaffected regions. The borehole module within GMS, which permitted the placement of boreholes, was used to determine the depth of the first (uppermost) material layer. GMS served as a rudimentary CAD tool to create the containment facility to a uniform thickness and height. The meshing capabilities within GMS were then utilized to generate a prismatic mesh (that is, a surface triangulation was extruded in layers along the z-axis). Boundary conditions were established near the shoreline, at the base of the material layer, and along the walls of the containment facility. The mesh and its associated boundary conditions were then passed to the 3D groundwater solver to generate steady-state results under minimal, average, and maximal facility loading characteristics on the ERDC HPC SGI Origin 3900 system. Results of the analysis were visualized in GMS as contour maps and velocity maps, with a focus upon the proposed facility and its immediate environs. The final determination was that the facility as proposed was inadequate to prevent saltwater contamination of the nearby freshwater aquifers.

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Stochastic hydrogeology: what professionals really need?

Authors: Philippe Renard

During the last decades, stochastic hydrogeology became an important field of research. This is illustrated by the number of textbooks that have been recently published on this topic and by the number of publications that one can find in the most renewed international journals. However, there is a debate about the lack of applications of the methods when dealing with engineering applications. I believe that the debate is still very open. Diverse opinions co-exist both on the degree of applications and on the degree of applicability of the methods. The aim of this presentation is therefore to discuss what is the status of stochastic hydrogeology in 2008. More precisely, I will discuss a number of reasons that may hinder the application of these techniques to real case applications. These reasons are technical, political, educational and economical. I argue that if the groundwater modellers are convinced that uncertainty needs to be accounted for when dealing with real applications, then the whole community needs to work at all these different levels.

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Stochastic Langevin Model for Flow and Transport in Porous Media

Authors: Alexandre M Tartakovsky, Daniel M Tartakovsky, Paul Meakin

A new stochastic Lagrangian model for fluid flow and transport in porous media is described. The fluid is represented by particles whose flow and dispersion in a continuous porous medium is governed by a Langevin equation. Changes in the properties of the fluid particles (e.g. the solute concentration) due to molecular diffusion is governed by the advection-diffusion equation. The separate treatment of advective and diffusive mixing in the stochastic model has an advantage over the classical advection-dispersion theory, which uses a single effective diffusion coefficient (the dispersion coefficient) to describe both types of mixing leading to over-prediction of mixing induced effective reaction rates. The solutions of advection-dispersion equations and stochastic advection-diffusion equations were compared for the transport of a conservative tracer, for multi-component reactive transport and for a RT instability. The simulation results show that for large Peclet numbers, commonly observed in field-scale transport, the advection-dispersion equation overestimates the solute mixing and produces artificially smooth concentration profiles. As a result, the advection-dispersion equations significantly overestimate the concentrations of the product of chemical reactions. In the case of RT instabilities, the advection-dispersion equation produced fronts with a lower effective fractal dimension and lower propagation rate than the stochastic advection-diffusion equations. Proposed stochastic flow model is based on a Langevin equation that is commonly used to represent random walk processes. In the same time, the stochastic flow model and random walk models differ significantly since the random velocities of the fluid particles satisfy the continuity equation while the velocities of random walkers (tracer particles) do not. The advantages of the stochastic flow model are: 1. Both molecular diffusion and chemical kinetics can be easily included via the stochastic advection-diffusion equation with appropriate source terms; and 2. Coupling between the flow and changes in the solute concentration field(s) occurs naturally in the model.

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Stochastic Multiobjective Management of Groundwater Supply Systems

Authors: Domenico Bau\'

A typical management problem associated with the development of groundwater resources involves the design of pumping schemes the maximize benefits while meeting a series of economical, technical and environmental constraints. Groundwater flow models combined with optimization algorithms are used to tackle this management problem, which is usually solved deterministically, that is, assuming perfect knowledge of the subsurface system. However, it is widely recognized that, due to scarcity of information on hydrogeological settings, parameter distributions, boundary and initial conditions, stochastic modeling approaches are often more appropriate. In general, since the implementation of a pumping strategy assessed based on uncertain hydrogeological parameters leads to a decision involving the risk of not meeting the design constraints, operations may be designed trough a multi-objective optimization framework that considers the tradeoffs between the benefit and the reliability of the groundwater supply system. In this work, an innovative stochastic multiobjective framework for optimizing the design and the management groundwater supply systems in the presence of parameter uncertainty is advanced. The objective is the determination of pumping strategies that minimize the total cost of the water supply system, while meeting a prescribed demand and minimize the probability of violating limitations imposed on aquifer drawdown. The fundamental components of the framework are: a three-dimensional finite element saturated flow model to calculate the aquifer response to pumping; a stochastic simulator of multivariate random processes to generate spatial distributions of the uncertain aquifer parameters, e.g. hydraulic conductivity; a niched Pareto genetic algorithm (NPGA) for the solution of unconstrained multi-objective optimization problems. A rigorous solution to this multiobjective optimization problem would require the NPGA to be combined with a stochastic groundwater flow model, used to calculate the management objectives as a function of any given pumping scheme. Because of the overwhelming computational effort involved, a “response surface” model must be introduced to estimate the objective functions. The response surface model used here stems from the development of matrices that relate the pumping rates for a number of potential well locations to the drawdown at the same locations. These “response matrices” are calculated from a series stochastic flow simulations using unit pumping rates at each candidate well. In the case of confined aquifers subject to most common boundary conditions, there exists a linear relationship between pumping rates and drawdown. In these instances, the response surface model obtained with this approach may thus be considered exact. In the investigated problem, two approaches are analyzed for addressing the tradeoff cost vs. reliability: in one case the reliability is estimated in terms of the probability of drawdown violation; in another, the reliability is assessed from the average intensity of drawdown violation. The analysis of the two approaches indicates that averaging violations can account not only for their frequency, as the probability of failure does, but also for the intensity with which they occur. Ultimately, the average drawdown violation method allows for considering less restrictive pumping policies.

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Structural organization of metadata catalogues in water research and management

Authors: Wolf-Dieter Otte, Mike Kasper

This paper investigates the structural organization of metadata as it is found in the field of water research and management. The methodology developed, organizes metadata in “metadata catalogues”. These catalogues reside in native XML databases (NXDs), which are used as the persistent storage medium. Individual NXDs are federated to form recursive virtual NXDs (VNXDs), which again can be federated with other NXDs as well as VNXDs. It will be shown, that this approach lends itself especially well to the fundamental principle of managing metadata in an environment, where data is sampled, stored and processed at many different geographic locations and under different jurisdictions. This is commonly the case in water research and management. However, the results presented are also applicable to many other scientific areas. Using the concepts outlined, an open source software package was designed and developed. This package contains a server component (NexusDB) as well as graphically enhanced client software (NexusClient). The presentation will show the utility of this software, in a practical demonstration.

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Structured uncertainty assessment in groundwater modelling

Authors: Anker Lajer Højberg, Jens Christian Refsgaard

Uncertainty assessment in groundwater modelling has evolved from being mostly research oriented to be standard in most groundwater studies carried out by consultancies. This trend reflects the increasing focus among water managers on the importance of assessing the uncertainties, and it is facilitated by uncertainty methods that are included in most sophisticated modelling software. These methods are almost entirely addressing the part of the uncertainty that can be statistically quantified, such as the effects of parameter uncertainty assessed by Monte Carlo simulations. However, the statistically quantifiable uncertainty comprises only a small part of the entire uncertainty space, and several studies have stressed that uncertainties in the conceptual model is often the predominant source of uncertainty in groundwater modelling. To include the various sources of uncertainty in a balanced manner it is important that uncertainty is considered throughout a groundwater study, and not just as an add-on to the modelling exercise. A structured uncertainty assessment should include three elements: 1. Identification of uncertainty sources. Here, all the sources of uncertainty need to be identified. This will typically include uncertainty on field data, on parameter values, on the conceptual model, on the approximations made in the numerical model and on the overall context of the modelling study (what is not included, e.g. climate change). Identification of the uncertainties is an ongoing process, starting with the formulation of the objectives and continuing throughout the model study. To embrace the entire uncertainty from a management perspective, it is crucial that the water manager and the concerned stakeholders participate in this process and that a common understanding is reached among these parties. 2. Characterisation of the uncertainty. The magnitude of the different uncertainties must be assessed – how certain/uncertain are we in a given quantity. An important aspect is that data stored in databases do generally only store a single value but hold no information on the data uncertainty. Although data may not be transferred directly to model setups due to scaling issues, it is vital that an estimate of the reliability of the data can be assessed. Furthermore, knowledge on the uncertainty in the calibration targets, like hydraulic heads and discharges, must be quantified prior to the model calibration and uncertainty assessments. Central to groundwater modelling is model conceptualisation, which is based on interpretation of all available data, and data uncertainty must thus be taken into consideration when a conceptual model is constructed. Particular important for groundwater modelling is the interpretation of the geological and hydraulic settings. Similar to the other data types it is critical that uncertainty in the geological data can be assessed. 3. Assessment of the effect of the uncertainty on the model prediction. This is commonly carried out by using the model to propagate the uncertainties to the final model results. Prior to this the relevant model simulations for the uncertainty assessment must be defined. Uncertainties critical to e.g. delineation of capture zones may be different from those important for groundwater-surface interaction, and the design of the uncertainty assessment is thus unique for each model study and should be based on both the assessments above, but also the specific modelling objectives and the requirements set up in a model study plan. While numerous methods have been developed on the assessment of the statistical uncertainty, the quantification of the conceptual uncertainty still poses major challenges. The procedure will be illustrated by an ongoing uncertainty assessment of results from the Danish national hydrological model.

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Synthesis of hydrologic data reveals rainfall-runoff relationships and examines watershed-scale changes

Authors: James R. Hunt, Deborah A. Agarwal, Catharine van Ingen

The Russian River basin in California is typical of many watersheds on the fringe of expanding metropolitan regions with competing demands for water from municipal, agricultural, recreational, and environmental constituencies. The Russian River basin is convenient for hydrologic analysis because there is limited water imported into the watershed and minimal water exported to other watersheds. Over time, the basin has undergone alteration by the construction and operation of flood control and water supply reservoirs, extensive gravel mining in the flood plain, deforestration, channelization, increased agricultural activity largely in the production of wine grapes, and an expansion in residential population in urban and rural settings with their own water withdrawals and releases. Within this context of a continual change in land use practices there is the added pressure to restore salmonid fisheries that have declined substantially. Alteration of the hydrologic cycle is one of the factors attributed to the decline in migratory fish populations. This leads to the question whether changes in the hydrologic response of a complex watershed can be quantified from archival data at a level appropriate for resource managers? The hydrologic record within the Russian River watershed is extensive , but tools for analysis have been limited. On-Line Analytical Processing (OLAP) technology enables organized and efficient browsing of large heterogeneous scientific datasets via the Internet. Using OLAP technology, hydrologic and meteorologic data from this and other California watersheds are organized into a data cube using the primary dimensions of time, place, and data type. The resulting data cube permits a rapid assessment of data availability, aggregation along dimensions, and the ability to download the needed data for analysis. In a data cube constructed for California watersheds, runoff and rainfall data aggregation along the time dimension enables examination of water year rainfall-runoff relationships for the Russian River watershed and sub-watersheds over time periods of decades. This examination has revealed a relatively simple relationship between water year rainfall depth over the watershed and water year runoff depth over the watershed with runoff depth equal to rainfall depth minus approximately 450 mm. This relationship holds for watersheds that span two orders of magnitude in area from 41 square kilometers up to 3500 square kilometers. The difference between rainfall and runoff is the watershed-scale evapotranspiration largely dominated by plant transpiration since there is limited free water surface evaporation in these watersheds. Hydrologic data analyses from multiple watersheds and precipitation records have revealed a relatively simple relationship within the Russian River watersheds that has not changed over the 60 plus years of data records even though the watershed has undergone substantial alteration in water storage and land use. The constancy of this relationship is likely a consequence of the development of terrestrial ecosystems in response to the topography and long-term precipitation records. This relationship can thus be used in a predictive mode to evaluate changes in precipitation expected from various climate change scenarios. Additional hydrologic data synthesis is enabled by the data cube for runoff dynamics at daily and shorter time intervals, such as daily water temperature dynamics that impact fisheries, and river sediment transport at time intervals of every 15 minutes. The availability of OLAP tools for environmental data analysis enables highly heterogeneous hydrologic data to be easily integrated together and contribute to the synthesis that is needed in current resource management applications and in anticipation of climate change impacts.

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Temporal Moments in Geophysical Monitoring of Salt-Tracer Experiments

Authors: Davina Pollock, Olaf A. Cirpka

Electrical Resistivity Tomography (ERT) has been successfully used to image the movement of salt tracers in controlled experiments. So far, the analysis of actual experiments has been restricted to computing spatial moments of the solute plume. Even on this crude level, physically impossible results have been obtained. In particular, decoupled geoelectric inversion does not guarantee conservation of solute mass. Besides this shortcoming, hydrological analysis of salt-plume images obtained from independent ERT inversion is disadvantageous because of the amount of intermediate data produced and the spatially correlated uncertainty of the concentration estimates. We suggest using temporal moments of electrical-potential perturbations as data for fully coupled hydrogeophysical inversion. We have derived moment-generating equations to compute these temporal moments without the need of transient-transport calculations. We apply the continuous adjoint-state method to compute the sensitivities of electrical-potential temporal moments on the hydraulic conductivity throughout the domain for given boundary conditions. No intermediate sensitivities are computed. The moment-generating equations require linearization of the Poisson equation. While the effects of linearization on the zeroth and first temporal moments are significant when considering easy-to-detect tracer concentrations, they are negligible for the ratio of the first to the zeroth moment, i.e., the characteristic time at which a potential difference is measured at an electrode pair due to the tracer test. We intend to implement the moment-generating equations and the scheme for evaluating sensitivities in an inversion scheme to estimate the hydraulic-conductivity distribution using geostatistical regularization, and to apply it to tracer-test data obtained in a quasi two-dimensional sandbox.

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Temporally and spatially adaptive time integration methods for Richards' equation

Authors: Sarah E. Gasda, Matthew W. Farthing, Christopher E. Kees, Cass T. Miller

Richards' equation is the most common model used to describe water movement through unsaturated porous media and has a wide range of applications in hydrology. Despite its popularity, the computational challenges of solving Richards' equation are significant because it is a non-linear parabolic partial differential equation that is characterized by sharp fronts of infiltrating water that persist in both space and time. Conventional numerical methods traditionally handle sharp fronts by finely-discretizing the entire spatial domain, which leads to an accurate, yet computationally inefficient, numerical solution. Thus, the importance of Richards' equation has spurred many advances in numerical methods to maintain or increase accuracy of the solution while also increasing the computational speed of the method. In particular, time integration techniques have been improved to allow for variable-order, variable-step-size integration methods that are reliable and efficient. These methods can be applied to spatially discretized systems through the use of the method of lines approach, further improving the robustness of temporal approximation methods. To achieve efficient resolution of sharp fronts and reduce spatial error, spatial discretization methods are now able to dynamically adapt grids to provide higher resolution in the vicinity of a sharp front and coarser resolution in smoother areas of the solution. The improvements in the solution accuracy and computational efficiency have been substantial over standard methods. The focus of this work is on improved temporal approximation techniques within spatially and temporally adaptive solution algorithms. Specifically, we consider the behavior of variable-order, variable-step-size multistep integrators for method of line simulations with dynamically changing grids. We then examine the impact of alternative error indicators, adaption heuristics, and startup procedures on efficiency and robustness for a series of variably saturated flow problems with sharp fronts and dynamic boundary conditions.

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The applicability of calibration-constrained predictive uncertainty analysis techniques to strongly non-linear models with high parameter dimensionality

Authors: Elizabeth Keating, John Doherty, Jasper A. Vrugt, Andrew Wolfsberg

A numerically-intensive process-level model has been developed to simulate groundwater flow below Yucca Flat at the Nevada Test Site, where the majority of U.S. underground nuclear tests were conducted (more than 600 tests). Underground testing had a profound impact on pore-water pressures; simulating the spatial and temporal manifestations of these pressure changes near each test is essential to model performance, but requires long run-times (hours) and high parameter dimensionality (more than 250 parameters). The relationship between model parameters and simulated observations and predictions are, in many cases, strongly non-linear which makes both model calibration and uncertainty analysis very difficult. The large parameter dimensionality and long run-times precludes the use of statistically-robust methods such as Markov Chain Monte Carlo simulation. Instead, we utilize a much more numerically efficient method employed by PEST, null-space Monte Carlo analysis, which generates a suite of parameter combinations, all satisfying established calibration criteria. These parameter combinations are then used to produce a range of finite-probability model predictions, specifically, the cumulative enhanced groundwater flux out of the saturated volcanics due to 30 years of underground nuclear testing. The question remains, however, how robust are the uncertainty estimates provided by this method? To address this question, we have developed a heuristic model with very fast run-times (1-2 seconds) which replicates key aspects of the process model; in particular, the relationships between model inputs (testing-induced pressurization and aquifer properties) and outputs (hydrographs at known wells). Using the same parameter and calibration datasets available to the process model, we use both PEST and adaptive Markov Chain Monte Carlo simulation (the DREAM algorithm) to estimate parameters and their associated (non-linear) uncertainty. We compare the statistics of the parameter distributions estimated in this way to the estimates provided by PEST for the process model, and to the results provided by both methods for the heuristic model. Key differences were noted for a sub-set of model parameters, which allows us to understand the strengths and weaknesses of using PEST for this application and for using a heuristic model to estimate parametric uncertainty for a more detailed process model. In particular, some sectors of parameter space were identified by DREAM but missed by PEST. We estimate the impact of these omissions to our prediction uncertainty analysis by sampling these sectors and calculating associated predictions with the numerical process model. In this way, we measure the error associated with using the numerically-tractable method implemented in PEST for this application.

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The Applicability of Hybrid-Optimization Techniques for Solving the Plume Containment Problem

Authors: Genetha Gray, Katie Fowler, Josh Griffin, Matt Taddy

Tackling water resources management problems routinely requires the pairing of subsurface simulators and optimization algorithms. Unfortunately, this pairing can introduce a number of obstacles to obtaining reasonable solutions. The objective function and constraints rely on output from the simulator, and the simulator often requires the numerical solution to a system of nonlinear partial differential equations. Various assumptions can be made to simplify either the objective function or the physical system so that gradient-based methods apply, however the incorporation of realistic objection functions can be accomplished given the availability of derivative-free optimization methods. In this work, we describe a derivative-free "hybrid" approach to such problems. Each optimization technique has inherent strengths and weaknesses. Hybridization allows for the combination of the beneficial elements of multiple methods. For example, consider two methods A and B where method A is capable of handling noise and undefined points and method B excels in smooth regions with small amounts of noise. In this case, method A may be unacceptably slow to find a solution while method B may fail in noisy or discontinuous regions of the domain. By forming a hybrid, method A can help overcome difficult regions of the domain and method B can be applied for fast convergence and efficiency. Such an approach seems particularly suited to water resources management problems where the objective function is often non-smooth or discontinuous and the feasible region is usually disconnected. In this talk, we will specifically examine an algorithm which combines statistical emulation via treed Gaussian process with pattern search optimization. In previous work, we showed that the resulting method enabled robust local optimization more efficiently and effectively than either method on its own for a series of test problems as well as for a computer model calibration problem. Here, we will demonstrate the applicability of our hybrid method to a plume containment problem that was proposed in the literature specifically for benchmarking purposes, and has already been used for the comparison of a variety of derivative-free optimization algorithms. The hydrological setting is an unconfined aquifer and the objective function and constraints are nonlinear and discontinuous. We present promising numerical results as well as reduced computational costs. In addition, we will describe how the treed Gaussian process can be used as a post-processing and analysis of convergence tool to increase insight into the problem.

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The Application of Chaos Ant Colony Optimization Algorithm in Reservoir Optimal Operation

Authors: zhiliang wang, wenxue pan

The hybrid algorithm based on the chaos-optimization algorithm and the ant colony algorithm is proposed in this study. It is a method to solve the reservoir optimal operation. According to the randomicity, and ergodicity of chaos, the hybrid algorithm effectively improved the computing efficiency, and made it uneasy to evolve stagnates and solved the local optimization problem by searching all chaos variable and passing all statuses. Also, utilizing the advantage of positive-feedback information of ant colony algorithms, this new methodology improves the blindness of chaos searching and enhances the searching efficiency. The result indicates that the algorithm is very efficient and can seek the global-optimization points by the case study.

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The effect of viscosity ratio on immiscible viscous fingering in model porous networks

Authors: Paul R. Tortora, Shelley Anna, Martin Ferer, Grant Bromhal, Duane H. Smith

Viscous fingering takes place during immiscible drainage in porous media when the injected fluid is less viscous than the displaced fluid. The fingering patterns depend on several flow conditions and can significantly affect the efficiency of injection/production processes such as carbon sequestration, oil recovery, and aquifer remediation. One of these flow conditions is the ratio of the viscosity of the injected fluid to that of the displaced fluid. When the viscosity ratio is near unity the displacement pattern forms a stable front, and as the viscosity ratio decreases the pattern crosses over into viscous fingering. In this paper, we present the results of experiments in rectangular 2-dimensional model porous networks and the results of 2-dimensional pore-level simulations to demonstrate this effect. The fractal dimensions of the experimental results are determined using box-counting and analysis of saturation profiles as a basis for comparison with the results of the pore-level simulations and statistical models. Finally, we present x-ray computed tomography scans of fluid displacements in sandstone cores to demonstrate invasion patterns in real geologic samples. The microchannel networks used in the experiments are fabricated using soft lithography and consist of square grids of random-width microchannels with their intersections being pores. This well-defined geometry was selected to investigate the fundamental aspects of fluid displacements. Chen and Wilkinson (1985) demonstrated via experiments and computational simulations that viscous fingering patterns are strongly influenced by the distribution of throat diameters in a porous medium: a narrow distribution of diameters causes the injected fluid to form dendrites, and a wide distribution of diameters causes fingers of the invading fluid to branch and form fractal patterns as in naturally occurring porous media. These authors defined a randomness parameter for cylindrical throats ranging between 0 (for a single throat diameter) and 1 (for a very large range of throat diameters). A similar parameter may be defined for the rectangular throats present in our 2-dimensional experiments. For our networks, the value of the randomness parameter is approximately 1/3, which is the highest value possible given the limits of our fabrication methods. The results of pore-level simulations are compared with the experimental results on the basis of the fractal geometry of the invasion patterns obtained through image analysis. Here, two analytical methods are used: box counting and the analysis of saturation profiles. Box counting is used to obtain the fractal dimensions of single images. Saturation profiles are plots of the volume fraction of injected fluid as a function of distance from the injection point, and are a function the fractal dimension. Multiple saturation profiles are fit to this function so that the fractal dimensions of data ensembles may be determined. Several different viscosity ratios are obtained experimentally by injecting water into networks saturated with oils with different viscosities. All experiments are performed at the same capillary number. The experimental results demonstrate the crossover from stable displacement to viscous fingering as the viscosity ratio decreases as well as the dependence of the fractal dimension on the viscosity ratio. Corresponding results of the pore-level model are also obtained. These results for immiscible flows are similar to those obtained from pore-level simulations by Stevenson et al. (2006) for miscible flows. REFERENCES: Chen, J.-D. and Wilkinson, D., (1985), Pore-scale viscous fingering in porous media, Physical Review Letters 55:1892-1895 Stevenson, K., Ferer, M., Bromhal, G.S., Gump, J., Wilder, J. And Smith, D.H., (2006), 2-D network model simulation of miscible two-phase flow displacements in porous media: effects of heterogeneity and viscosity, Physica A 367:7-24

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The Effects of Coarsening on Mass-Conservation for a Fully Adaptive Implementation of Richards' Equation

Authors: Godfred Yamoah, K. R. Fowler, Owen Eslinger, Christopher kees, Jackie Hallberg, Stacy Howington

Richards' equation (RE), a partial differential equation which can be nonlinear for certain physical parameters, is often used to model flow in variably saturated media. Solutions to RE are commonly obtained using finite difference or finite elements with implicit temporal integration. Spatial and temporal adaptive methods have been shown to improve the efficiency as well as the accuracy of the numerical solution, especially in simulations that are characterized by sharp moving fronts in the domain in space and time. Difficulties to these adaptive methods still remain however and include managing the discretization scheme to preserve and accuracy of the solution as well as to conserve mass, in particular during the mesh coarsening. Many schemes simply delete nodes during coarsening which often lead to mass conservation errors because values of the adjacent nodes of the deleted nodes are not adjusted to preserve mass over the coarsened grid. Also while numerous adaptive discretization schemes adaptive schemes to RE exist independently for spatial and temporary adaptive schemes, not much work has been done with regards to joint spatial and temporal schemes for RE. We first implement three spatial adaptive schemes in 1D, and combine the schemes first with a heuristic time stepping method and then with an adaptive temporal scheme based on error control. The spatial schemes involve three different coarsening methods, one in which nodes are simply removed, another based on a mass conservative formula and a third method based on an optimization scheme. We will present numerical results comparing the different joint schemes on two infiltration simulations for sand silt and clay. We measure the performance of the methods based the accuracy of the solution, the work done and the amount of mass conserved. Our motivation is the Adaptive Hydrology Model(ADH), being developed by the US Army corps of Engineers, for solving surface and ground water flow problems

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The effects of uncertainty on a coastal aquifer management problem

Authors: Karen L. Ricciardi, Ann E. Mulligan

Management of coastal aquifers involves the use of numerical models to predict the effects of pumping on the hydrologic properties of the aquifer. Of great importance in these types of management problems is the correct prediction of the saltwater-freshwater interface to avoid saltwater intrusion issues. Often municipalities place upper limits on the allowable amount of pumping to avoid such issues. When these limits are based upon deterministic groundwater flow models they may be set conservatively high in order to avoid the risks associated with the uncertainty of the groundwater model. This research investigates the effects of the uncertainty in a groundwater flow model on the prediction of the location of the saltwater-freshwater interface. Using the results of this investigation a groundwater management system is developed that takes into consideration the uncertainty in the model. This analysis is applied to a hypothetical model based upon the hydrologic conditions of the Truro aquifer located on the Lower Cape Cod Aquifer in Massachusetts. In the proposed groundwater model the location of the salt-water interface is approximated using the Ghyben-Herzberg relation. An iterative scheme is used to calculate the hydraulic head of the free surface of the unconfined fresh water aquifer as a function of the depth to the saltwater-freshwater interface. The steady state solution to the groundwater flow model is used in this approach resulting in a conservative calculation of the depth of the saltwater-freshwater interface. The uncertainty in this calculation is examined by applying this iterative scheme to multiple models of the coastal aquifer system differentiated by their hydraulic conductivity fields. The hydraulic conductivity fields are spatially variable fields generated by using the geostatistical software GSLIB. The uncertainty in the saltwater-freshwater interface in the model is then used to examine the risk of saltwater intrusion into pumping wells in an existing applied management system. By applying optimization techniques a new conservative management system that takes into account the uncertainty in the model is developed. This new groundwater management system is one that minimizes the risk of saltwater intrusion into pre-existing pumping wells while meeting the supply demands of the community. Through this project the effects of uncertainty on saltwater intrusion problems are explored.

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The Hybrid Finite-Element Mixing-Cell method: a new flexible method for large scale groundwater modelling

Authors: Orban Philippe, Brouyère Serge, Wildemeersch Samuel, Couturier Julie, Dassargues Alain

Interest of end-users and policy makers for understanding and managing water systems at the regional scale has increased for years. At this scale, groundwater models of different complexity ranging from black-box models to physically based distributed models have been used in various hydrogeological conditions. Black-box models, such as transfer functions, have been applied for example to model groundwater in large scale hydrological models, to model karstic systems, in particular for the interpretation of isotopic data. Their concepts are simple and attractive because they require relatively few data. The main drawbacks are however that modelling results are not spatially distributed and their predictive capability is questionable due to the semi-empirical nature of process descriptions. On the contrary, due to a more advanced description of ongoing processes, physically-based distributed models are expected to have better predictive capabilities than black-box models. However, because such models require more data, they are generally applied for case studies that are better characterized from a hydrogeological point of view, for which the distribution of water levels or solute concentrations in the groundwater systems are needed. For large-scale modelling purposes, black-box models and physically-based distributed models have both proved their utilities and have their own justifications, advantages and disadvantages. However, few attempts have been made to combine the advantages of these two categories of approaches in a unified modelling application. A new flexible modelling approach, the Hybrid Finite-Element Mixing-Cell method (HFEMC), has been developed that allows combining in a single model, and in a fully integrated way, different mathematical approaches of various complexities for groundwater modelling in complex and large scale environments. This method has been implemented in the groundwater flow and solute transport numerical code SUFT3D. The approach has been first tested and illustrated using basic and advanced “synthetic” examples that allow validating and discussing its advantages over existing modelling concepts. The HFEMC approach is now applied for the development of a large scale groundwater flow and solute transport model in different groundwater basins in Belgium.

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THE NEED FOR A COMMUNITY HYDROLOGIC MODELING PLATFORM

Authors: Larry Murdoch, Jay Famiglietti, Venkat Lakshmi, Richard Hooper, Stephen Moysey, Scott Brame

Hydrologic models play a key role in both the advancement of hydrologic science and the predictive contributions that hydrology makes to society. Despite their importance, the development of hydrologic models has been limiting the hydrology community in several significant ways. Widely available hydrologic models typically represent processes across a limited set of domains (e.g. groundwater, unsaturated zone, rainfall-runoff, channel hydraulics, land surface-atmosphere, wetlands, lakes, etc.). However, research interests are drawn to interfaces between domains, or to processes that are poorly represented by available models. Research codes are developed to address these processes, but most of these codes never leave the computer where they were developed. Results from research codes are published, but the capabilities these codes provide remain largely inaccessible. Faced with the situation outlined above, many research hydrologists develop models to explain the results of their own experiments because they don't have access to models with the necessary capabilities. A significant time investment is required first to learn, and later to write these models. This investment is needed to explain experimental data and complete a research project, but the resulting model is rarely used by others so much of its potential is never realized. This is an inherently inefficient system, but researchers must either make the considerable intellectual investment in developing their own models or relinquish the scientific flexibility this affords. We suggest that scientific progress has been slowed by these inefficiencies, and that new approaches could lead to advances throughout the field of hydrology. CUAHSI is proposing that a new generation of simulation capabilities should be pursued to support and inspire scientific understanding in hydrology and associated disciplines. The vision is that this effort should provide an optimal environment for developing, sharing, and publishing capabilities to simulate hydrologic processes. Some of the potential capabilities and goals of the next generation should include: 1. Represent physics associated with all terrestrial water. 2. Accommodate a wide range of scales; from pore to continent. 3. Flexibility to represent many physical, chemical and biological processes. 4. Ability to advance and modify capabilities using input from the community. 5. Easy to use and readily available to community. 6. Take advantage of modern and emerging computing capabilities. 7. Couple with ocean and atmospheric circulation models. 8. Exchange data with the CUAHSI Hydrologic Information System (HIS). 9. Estimate model parameters and characterize uncertainty from large data sets. 10. Represent stochastic processes. Implementing the capabilities outlined above would require several major software packages with distinctly different functionality: 1. Forward package to represent distributed hydrologic processes across scales, 2. Inverse package with parameter estimation and optimization schemes, 3. Stochastic package with general geostatistical capabilities 4. Visualization package with general graphical and data display capabilities 5. Data access package to interact with HIS. These packages would be supported on a common platform, which we term a hydrologic modeling platform. There are a variety of options for the architecture of a hydrologic modeling platform and associated packages, and it will be important for the community to decide on which options best serve its needs before construction begins. CUAHSI has initiated an effort to evaluate these options and a status report will be presented at the conference. The evaluation currently includes plans for open workshops designed to review community needs and interests in late 2008 or 2009. Consult http://www.cuahsi.org for opportunities to get involved with the hydrologic modeling platform workshops.

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The Use of Surface-Water Fluctuations and Aquifer Properties to Evaluate Contaminant Fate and Transport in Groundwater.

Authors: Jonathan C. Johnson PhD

The interaction between surface water and groundwater is inherently not a steady phenomenon. Variability in the potential associated with the surface water body can result in hydraulic gradients into or out of the adjacent aquifer. Since dispersion is related to the absolute value of the velocity, changes in sign for the hydraulic gradient result in enhanced dispersion within the aquifer near the surface water body. Contaminant transport under these conditions has been explored for the evaluation of the influence of tides on transport in an adjacent aquifer. However, analysis has been limited to a single frequency “signal” associated with the surface water body. In this paper, we extend the generalized approach that takes the Fourier transform of the surface-water body “signal” to evaluate the flow field. Combining this signal with information about the regional flow gradient and aquifer properties, the velocity and direction of flow within the aquifer can be determined. This technique allows evaluation of aquifer interactions in more complex environments such as a streams and rivers. Our results show that 1) The surface-water fluctuations affect the contaminant fate and transport to a limited distance within the aquifer; 2) the maximum distance of influence on fate and transport in the aquifer can be evaluated directly from the aquifer properties, regional flow gradient and the “signal” representing the surface water body; 3) The enhanced dispersion can be represented as a function of distance from the surface water body; and 4) the first-order decay term is also affected by the velocity fluctuations associated with this “signal”.

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Theoretical analysis of CO2 plume vertical migration in a stratified heterogeneous porous media

Authors: Mohamed HAYEK, Emmanuel MOUCHE, Claude MUGLER

The migration of a CO2 plume in porous media can be described by the fractional flow model, consisting of a saturation equation for the non-wetting phase (CO2) and an equation for the total velocity. If capillary forces and CO2 dissolution are neglected, then the saturation equation is a non-linear hyperbolic conservation law known as the Buckley–Leverett equation. The solution of a Riemann problem for the Buckley–Leverett equation is well known if gravity is neglected and if the porous medium is homogeneous. Whereas, there have been few studies when gravity is not neglected and the porous media is heterogeneous. In this work, we analyse the dynamics of a CO2 plume in a vertical (i.e. with gravity) stratified heterogeneous porous media. First, we consider the homogeneous case; the solution is characterized by a composition of shocks and rarefaction waves. Second, we study the behaviour of the solution when the plume reaches an interface between two different permeability regions. The continuity of flux must be imposed at the interface at every moment, which implies a discontinuity of CO2 saturation. Then, depending on the flux value, the plume either accumulates or/and passes through the interface. Finally, we analyse the behaviour of the plume in a stratified heterogeneous porous media. We explain mathematically the possible accumulation of CO2 under the layers. A semi-analytical solution is derived in the case of periodic stratified porous media of Sleipner type. In such case, the lowest layer filters the CO2 (i.e. the CO2 accumulates only under the lowest impervious layer) and the plume must propagate with discontinuity in saturation at each interface. Comparisons between semi-analytical solutions and numerical results are presented.

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Three-dimensional hydrogeophysical zonation of a gravel aquifer in the vicinity of the Thur River, Switzerland

Authors: Joseph Doetsch, Niklas Linde, Ilaria Coscia, Laurent Marescot, Jacques Ernst, Alan Green, Baptiste Dafflon, Klaus Holliger

A multidisciplinary research team is currently investigating the hydrological, ecological and biochemical effects of river restoration using field-based studies at the Thur River in northern Switzerland. We describe the results of a hydrogeophysical pilot study of a producing gravel aquifer in the vicinity of an unrestored section of the river. Our objectives are to estimate the spatial variability of hydrogeological and geophysical properties of the river sediments and derive a three-dimensional zoned representation of the subsurface as a basis for future hydrogeophysical inverse modeling. Eventually, we intend to construct a hydrological model that can predict future interactions between river water and groundwater using temporal variations of river-water electrical conductivity and level measured at a nearby river station. The 7-m-thick gravel aquifer is being accessed through four 11.4 cm fully-slotted PVC-cased boreholes located at the corners of a 5 x 5 m square approximately 10 m from the river. Geophysical borehole logging (natural gamma, gamma-gamma, and neutron-neutron) yields high-resolution 1D information in the vicinity of the boreholes, whereas crosshole seismic, radar and electrical resistivity surveys map the physical properties between the boreholes. The grain-size distribution and key petrophysical parameters are being determined from the retrieved cores. Our crosshole seismic and radar data are being inverted jointly using a non-linear traveltime tomography algorithm that incorporates stochastic regularization operators based on analyses of flowmeter data, borehole logs, and our geological understanding of the site. Coupling between the models is achieved by employing cross-gradient constraints that enforce structural similarity. We are also inverting the crosshole radar data using a 2D full-waveform inversion code that provides high-resolution models of dielectric permittivity and electrical conductivity. To analyze the various models based on the individually and jointly inverted geophysical data, we are further developing classification and clustering methods that will supply zoned representations of the subsurface. Each zone will be characterized by the mean values and spatial variabilities of the inverted parameters (seismic velocity, relative permittivity, and electrical conductivity).

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Three-dimensional mixed-wet random pore-scale network modeling of relationships between interfacial area, capillary pressure, and saturation

Authors: Behrooz Raeesi, Mohammad Piri

Interfacial area between different phases is among most important parameters for multicomponent multiphase transport processes in porous media. We use a three-dimensional mixed-wet random pore-scale network model to investigate the relationship between interfacial area, capillary pressure and saturation in two-phase drainage and imbibition processes in systems of varying wettability. The model is a three-dimensional network of interconnected pores and throats of various geometrical shapes. It allows multiple phases to be present in each capillary element in wetting and spreading layers, as well as occupying the center of the pore space. Each displacement is modeled as a change in fluid configurations. Then a series of displacement steps in each pore or throat are combined to simulate different flow processes. Several different random networks that represent the pore space in various rocks (e.g. Berea sandstone) are used in this study. A robust displacement-based clustering algorithm is used to track the continuity of each phase-location. Contact angle hysteresis is also taken into account by using receding and advancing oil/water contact angles for drainage and imbibition processes, respectively. We allow the wettability of the surfaces contacted by oil to alter after primary drainage. We model primary oil drainage, water-flooding and secondary oil injection for mixed-wet conditions. Piston-like, snap-off, pore-body filling and layer collapse/formation are the displacement mechanisms that we utilize to simulate the abovementioned processes in systems of varying wettability. We use thermodynamically consistent threshold capillary pressures as well as geometrical criteria to select the most favorable displacement mechanism and associated fluid configuration at every step. The total interfacial area for pores and throats are calculated at different capillary pressures and saturations when the system is at capillary equilibrium. They include contributions from the arc menisci between the bulk and corner fluids (AM), and from the main terminal menisci (MTM) between different bulk fluids. We also investigate the effects of phase entrapment on interfacial area by performing water injection into systems of varying initial water saturation. Initial water saturation directly, in water-wet systems, affects the amount of residual oil saturation. We perform primary drainage to reach different oil saturations and then inject water. This generates different amounts of residual oil saturation at the end of water-flooding. We also define several systems with varying wettability (e.g., strongly water-wet, weakly water-wet, weakly oil-wet and strongly oil-wet). We then investigate hysteresis in the relationship between the interfacial area, capillary pressure and saturation in these systems. Furthermore, we investigate the relationships when secondary oil injection is carried out with different initial oil saturations. We examine the theoretical conjectures in which the definition of an extended constitutive relationship between capillary pressure, saturation, and interfacial area eliminates hysteresis between drainage and imbibition.

Three-Dimensional Modeling Of Gas Migration In A Deep Low/Intermediate Level Waste Repository (Switzerland)

Authors: Rainer Senger, Keni Zhang, John Avis, Paul Marschall

Gas migration in a low/intermediate-level waste (L/ILW) repository is a critical component in the safety assessment of proposed deep repositories in low-permeability formations. In L/ILW repositories, anaerobic corrosion of metals and degradation of organic materials produces mainly hydrogen and methane. The generation, accumulation and release of these gases from the disposal system may affect a number of processes that influence long-term radiological safety of the repository. After closure, the repository performance with respect to gas migration and pressure buildup will be affected not only by the two-phase properties of the EBS and surrounding host rock, but also by a variety of other geological, geotechnical, and waste-related factors. The Swiss National Cooperative for the Disposal of Radioactive Waste (NAGRA) has conducted a feasibility study for a generic L/ILW repository in a low-permeability claystone formation. The repository consists of as many as seven parallel caverns which are sealed off from a single access tunnel. Additional underground structures include a pilot cavern, an underground rock laboratory (URL), a ventilation shaft and a central area. In order to assess the risk of buildup of excess gas pressures in the backfilled emplacement caverns after repository closure, the development of a site-scale two-phase flow model was initiated. A further aspect was the optimization of the repository design as to avoid unacceptable gas pressures in underground structures (design of an “engineered gas release path”). The two-phase model used an integrated finite difference (IFD) mesh. Implementation of the tunnel and cavern geometry was simplified, representing the radial geometry by equivalent rectangular cross sections of the tunnels and caverns For the simulation of two-phase flow in a complex 3D model, the parallel version of the two-phase flow simulator TOUGH2_MP (Zhang and Wu, 2006) was used. The development of the 3D model geometry was automated using the visualization software mView (Calder and Avis, 2006). For this, mView was modified for nested gridding, allowing refinement near the underground repository and a coarser mesh in the far field. The resulting mesh was comprised of 299,844 elements. The pre-processor utility in mView was then used for generating the input files for TOUGH2. In addition, mView utilities were used to extract the elements and connections representing only the EBS from the entire model. This allowed performing sensitivity simulations to evaluate different dimensions and properties for the different EBS elements using a much smaller model grid (27,822 elements). The transient hydrodynamic conditions associated with the excavation of the tunnels and caverns, and subsequent waste emplacement and backfilling of the underground openings were modeled with the 3D model, representing initial partially-saturated conditions at atmospheric pressures in the EBS for the start of the post-closure period. Gas generation was assumed to start under partially-saturated initial conditions. The different gas components were represented by a single gas phase (air) using the TOUGH2 EOS3 module. The model results show that simulated pressures can vary significantly between different parts of the repository, indicating that after 1,000 yrs, the area of URL has still not reached hydrostatic conditions, whereas the repository cavern indicate overpressured conditions. The numerical simulation for the reference case was run on a Linux cluster with 24 CPUs (Intel Xeon CPU 5150 @ 2.66 GHz) and required 14,924 time steps for a total run time of 66.3 hours. The study demonstrated the feasibility of performing two-phase flow simulations using large 3D site-scale repository models by combining efficient mesh design and parallel computation capabilities. In addition, by extracting the EBS portion of the model, sensitivity simulations could be performed for optimizing the EBS design.

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Three-dimensional series solutions for regional multi-layer flow in sloping aquifers

Authors: James R. Craig, Sanders Wong

A Fourier series solution method is developed for simulation of regional three-dimensional multi-aquifer flow, where the anisotropic aquifer layers are parallel. The solution is predicated upon the assumption of a known water table surface elevation (typically assumed to be correlated to the topographic surface) and the application of no-flow boundaries at depth and along sides of the rectangular domain. A key feature of this solution which distinguishes it from alternative approaches (e.g., Wörman et al., Exact three-dimensional spectral solution to surface-groundwater interactions with arbitrary surface topography, Geophysical Research Letters, v33, 2006) is that the solution has multiple layers of arbitrary dip angle with respect to the vertical axis, extends all the way to the water table surface, and the water table may exist simultaneously in multiple aquifer layers. The solution is exact everywhere except at the water table surface, where the number of Fourier terms determines the accuracy to which the top boundary condition is met. All other boundary conditions and continuity conditions (head and flow continuity) at layer interfaces are met exactly. The solution is demonstrated with an application to the 17-layer regional fractured rock aquifer system beneath the Bruce Peninsula in Ontario, Canada.

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Three-dimensional Transport Modeling using the Finite Cell Approach

Authors: Ahmed E Hassan, Mohamed Attia, Hesham M Bekhit

Contaminant transport in the subsurface is impacted by a complex set of physical, chemical, and biological processes that cannot be decoupled if realistic field conditions are to be studied. These processes are governed by a coupled set of partial differential equations that should be developed and solved in three dimensions. Simulating these coupled processes in three dimensions is computationally demanding and may be prohibitive using traditional methods. A more efficient approach is developed using the finite cell approach, first developed by Sun (1999) in one dimensions, to model transport processes in three dimensions. The model is extended to deal with dual porosity systems and linear as well as nonlinear non-equilibrium reactive models. Preliminary results show that the model provides a potential tool for efficiently handling complex transport processes in three dimensions.

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TIME-ACCURATE, HIGH-ORDER SCHEMES FOR THE NUMERICAL SIMULATION OF NONEQUILIBRIUM MODELS OF MULTIPHASE FLOW IN POROUS MEDIA

Authors: Luis Cueto-Felgueroso, Ruben Juanes

The governing equations of multiphase flow through porous media are often expressed as a coupled nonlinear system: a near-elliptic equation for the pressure or the stream function and a quasi-hyperbolic equation for the saturation. After introducing a suitable spatial discretization, the resulting semidiscrete problem can be analyzed as a system of index-2 differential-algebraic equations (DAE). Furthermore, capillary effects and advanced non-equilibrium models induce higher order terms (eventually up to fourth order), which increase the complexity and stiffness of the numerical model. While a first-order coupling in time, such as the popular IMPES approach, is a widespread and computationally convenient option, the growing interest on high-fidelity simulations, which may shed light on fundamental aspects of porous media flows, requires the development of accurate and efficient high-order time discretizations that honor the fully coupled nature of the problem. We present high-resolution numerical simulations of advanced continuum models of multiphase flow through porous media. The spatial discretization is performed using a rational spectral method or a weighted essentially non-oscillatory (WENO) scheme, depending on the ability of the computational grid to resolve the complex features of the flow. The discretization in time is carried out by a spectral deferred correction method, which is suitable for stiff differential-algebraic equations. An interesting feature of the deferred correction approach is that our high-order time integration schemes are constructed from low-order approximations, and therefore existing first-order codes can be upgraded to high-order accuracy with reasonable additional coding effort.

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Toward Understanding the Role of Ground Water in Hydroclimate Using a Single Column Atmosphere Model

Authors: Jiming Jin , Norman L. Miller

A single column atmosphere model (SCAM) developed by the National Center for Atmospheric Research (NCAR) was used to investigate the role of the ground water level in hydroclimate. SCAM was driven by the Reanalysis data from National Centers for Environmental Prediction (NCEP)/NCAR for the 55-year period of 1948-2002 over the California Merced River Basin, and the lateral boundary conditions were updated every six hours. SCAM ran 55-year simulations independently at each of the 24 grid cells that cover the entire Merced watershed, where the major land cover is needle-leaf tree. The simulated results show that SCAM basically can reproduce the observed precipitation, 2 m height temperature, and streamflow. The statistical analysis based on the above simulations indicates that the water table is positively correlated with precipitation in winter. A similar correlation for precipitation and snow water equivalent (SWE) with the water table depth is seen in spring. In addition, surface temperature is found to play an important role in affecting water table depth in the Merced watershed in spring. The colder surface lifts up the water table by suppressing evaporation in this season, while the warmer surface lowers the water table by increasing evaporation. Meanwhile, a positive correlation between water table and runoff is very significant in spring. In summer, the higher (lower) water table produces stronger (weaker) evaporation, which significantly increases (decreases) precipitation, and such stronger (weaker) evaporation further results in colder (warmer) surface. In fall, the water table depth has a similar influence on evaporation to that in summer, but it is also positively correlated with runoff. Additional 30-year (1961-1990) SCAM simulations were performed at Russian Valdai station, where the land cover type is short grass. The observations measured at this station include high-quality atmospheric forcing data and ground water data. The Valdai simulations were fully evaluated with these observations and compared and contrasted with those for the Merced watershed to further understand the mechanisms of how groundwater level interacts with hydroclimate. In addition, the impact of the land cover difference (needle-leaf tree versus short grass) between these two sites on ground water level is identified.

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Towards a Complete Model of the Hydrologic Cycle: Idealized Simulations to Diagnose Land-Atmosphere Feedbacks

Authors: Jehan F. Rihani, Reed M. Maxwell, Fotini Katopodes Chow

Although previous studies have shown sensitivity of atmospheric processes to land surface and subsurface conditions, the extent of these interactions is not yet fully understood. Recent work used a coupled groundwater-atmospheric model to study interactions of groundwater, the land-surface and the atmosphere in a watershed in Oklahoma. In the current work, the goal is to use this coupled model to isolate these interactions in a set of idealized test cases to glean the effect of soil moisture heterogeneity and water table depth on dynamics of the atmospheric boundary layer under a variety of conditions. The coupled model combines ParFlow (PF), a three-dimensional variably saturated groundwater flow model, with a three-dimensional mesoscale atmospheric model, the Advanced Regional Atmospheric System (ARPS). The combined PF.ARPS is used to study idealized cases including tilted hillslope and sinusoidal terrain encompassing various representations of subsurface heterogeneity, geologic structure and atmospheric conditions. Offline spinups using ParFlow coupled to the Common Land Model (PF.CLM) are used to generate detailed soil moisture distributions for these idealized test cases. These spinup distributions are used to initialize both uncoupled ARPS and fully coupled PF.ARPS simulations of a typical diurnal cycle. Differences in the atmospheric dynamics resulting from a more accurate representation of the physical hydrologic processes are discussed.

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Translating climate-change uncertainties into impact risks--Are there 'best' choices of scenarios for detailed assessments?

Authors: Michael Dettinger

Projections of climate change in response to increasing greenhouse-gas concentrations are uncertain and likely to remain so for the foreseeable future. As more projections become available for analysts, we are increasingly able to characterize the probabilities of obtaining various levels of climate change in current projections. However, the probabilities of most interest in impact assessments are not specifically the probability of climate changes, but rather the probabilities (or risks) of various levels of climate-change impact. These risks can be difficult to estimate even if the climate-change probabilities are well known. The difficulty arises because, frequently, impact models and assessments are computationally demanding or time consuming of hands-on, human expert analyses, so that severe limits are placed on the numbers of climate-change scenarios for which detailed impacts can be assessed. Real-world examples will be used to show that, by applying several different \"derived distributions\" approaches for estimating the risks of various impacts from known climate-change probabilities to just a few impact-model simulations, the risks can be quantified along with indications of how accurate are the impact-risk estimates. The prospects for optimally selecting a few climate-change scenarios (from a larger ensemble of available climate-change projections) that will allow the best, most economical estimates of impact risks will be demonstrated for a simple but real-world case.

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Transport modeling of pesticides in soil porosity using Lattice Boltzmann simulations and 3D maps provided from X-ray computed tomography

Authors: Nadia ELYEZNASNI, Valerie POT, Irina Ginzburg, Alain GENTY

The Interest to Lattice Boltzmann method has been rapidly growing during recent years. The Lattice Boltzmann method is appealing because of its conceptual simplicity and many believe it has the potential to overcome, with a good accuracy and stability, some of the problems encountered with the conventional continuum-based CFD methods like incorporation of geometrically complex boundary conditions. The Lattice Boltzmann method describes a fluid at a molecular level and matches the Navier-Stokes equations as a second-order approximation of the exact microscopic mass and momentum conservation laws. Dropping the conservation of the momentum, the method is adapted for solving advection-diffusion equations and is well designed for studying transport of solutes in soils at the pore-scale level. Heterogeneities at the pore-scale level of physical (structure of soil), physico-chemical (adsorption/desorption) and biological origins do not appear explicitly in transport models of solutes in soils. Traditional mathematical models treat motion and adsorption reactions in soils by implicit description of heterogeneities (non-equilibrium transport models: two-porosity, multiple-permeability, kinetic adsorption). The identification of void space and simulation of reactive solute transport through it is a challenging task because of complicated geometry. Insight in structure of soil has been gained with the recent development in experimental techniques like computed tomography. to describe reaction kinetics by integrating the adsorption/desorption and degradation of pesticides by laws of first order. The lattice Boltzmann approach was chosen for its ability to simulate both water flow and transport of solutes tracers. We describe in a frame of the lattice Boltzmann two -relaxation-time (TRT) model (Ginzburg, 2005) the advection-diffusion process of solutes in Stokes flow and extend it for reaction kinetics, by integrating the adsorption/desorption and degradation of pesticides by laws of first order. In contrast with commonly used single-relaxation-time (BGK) model, the TRT model offers a consistent modeling of porous flow with no increase of computational cost. Reactivity of pesticides onto the solid constituents of soil is explicitly modeled through the identification of reactive sites: organic matter and organo-mineral phase. In our model organic matter and organo-minerals are described by different reaction kinetic laws. As a first step of our work we performed three-dimensional maps to describe pore space and localize reactive sites in soil. The maps were obtained by scanning soil cores using X-ray computed tomography . The soil cores (5 cm height and 5 cm diameter) were sampled in the surface horizon of a clay-loam soil provided from Feucherolles site (France). Resolution of the images was of 68 microns. Those tomograms have been explored as a serial of 750 surfaces by analyzing the Grey level of images. All surfaces were studied to detect differtent levels of density indicating different nature of soil constituents such as particulate organic matter, organo-mineral phase and void (porosity). We investigated also the pore space connectivity which is an important topological property of soil to model transport. The high quality of the tomographic images allowed to distinguish particulate organic matter from porosity and organo-mineral phases. After localization of diverse heterogeneities (pore space and reactive sites) in the 3D maps, all disconnected pores have been removed from the calculations to save computational cost and memory. The impact of adsorption/desorption heterogeneities has been tested and a comparison between hydrodynamic dispersion of inert solute tracer and reactive solute has been performed for homogeneous and heterogeneous adsorption for the original three-dimensional data.

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Transport of emulsions in porous media

Authors: Teamrat A. Ghezzehei, Andrea Cortis

Emulsions appear in many subsurface applications including bioremediation, surfactant-enhanced remediation, and enhanced oil-recovery. Modeling emulsion transport in porous media is particularly challenging because the rheological and physical properties of emulsions are different from averages of the components. Current modeling approaches are based on filtration theories, which are not suited to adequately address the pore-scale permeability fluctuations and reduction of absolute permeability that are often encountered during emulsion transport. In this communication, we introduce a continuous time random walk based alternative approach that captures these unique features of emulsion transport. Calculations based on the proposed approach resulted in excellent match with experimental observations of emulsion breakthrough from the literature. Specifically, the new approach explains the slow late-time tailing behavior that could not be fitted using the standard approach. The theory presented in this paper also provides an important stepping stone toward a generalized self-consistent modeling of multiphase flow.

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Two Dimensional Upscaling of Pressure and Mass Transfer Terms in a Two Phase Flow System

Authors: Juan P. Nogués, Jan M. Nordbotten, Michael A. Celia

In multiphase flow in porous media it is of great necessity to model systems at a coarse enough scale where computing power can give results in a timely manner. To model geological reservoirs at a fine enough scale to capture all the dynamics and heterogeneities the gridding required would put the number of cells in the order of tens of millions, which hinders the computer output time immensely. Though the computational power is one of the main drivers of upscaling techniques, this is not the only reason why upscaling should be done. After all, as pointed by Christie (1996), further increase in computation speed and effective use of parallel machines will remove the need for upscaling. However, one is faced with the fact that the system being modeled is but one geological realization of many possible realizations and that one needs to model a large number of cases in a monte-carlo fashion in order to predict the uncertainty of a problem. One of the most interesting applications in multiphase flow, which depends on the quickness of computation, is the modeling of the fate and transport of CO2 injection in deep geological formations. CO2 injection and storage is being proposed as a major mitigation option to reduce the greenhouse gas accumulation in the atmosphere (Pacala and Socolow, 2004). Therefore, it is important to understand how the CO2 will move and stay in these geological formations, or if there is the possibility of CO2 leakage, and if it does, where will it go. These issues call for a large computational effort with uncertainty bounds that can benefit from upscaling. Assuming that the same mass conservation laws and pressure equations are applicable at the coarse scale as in the fine scale, with correct effective parameters, we propose to study the upscaling constitutive relationships and geochemical reactions. In this study we concentrate in upscaling techniques that upscale capillary pressure and relative permeability by taking the saturation-weighted average approach but with a different definition of average pressure. The definition of pressure follows that presented in Nordbotten et al. (2007). In their paper they suggest a definition of macroscale pressure which takes into account the systematic subscale variation in saturation. In this study we will not dwell on the correct way of upscaling intrinsic permeability. Instead we choose a simple pressure solve method with permeameter boundary conditions and assume this is a good representation of the subgrid heterogeneities at the coarse scale. Likewise, the understanding of geochemical reactions in CO2 injection scenarios has been shown to be of crucial importance (Xu et al., 2003) because they explain how CO2 is naturally trapped and immobilized by the geologic formation. Unfortunately, upscaling mass transfer by volume averaging gives poor reaction rates at the coarse scale, which subsequently leads to the wrong representation of the fine scale (Li et al., 2005 and Meile and Tuncay, 2005). We try to overcome this problem by not volume averaging fine scale reaction rates, but instead by accounting for subgrid permeability values in order to account for the interface area along a saturation front where most of the mass transfer occurs. In order to study all these behaviors and techniques a two-dimensional semi-implicit model has been developed which solves for phase pressures and phase saturations implicitly and for mass fractions explicitly. The two mobile phases modeled are the CO2 rich non-wetting phase and the brine wetting phase. Salt is present as a static phase when it precipitates from the brine. The mass fractions calculated account for CO2 in the wetting and non-wetting phases, as well as the water in the brine and in the non-wetting phase. At the fine scale equilibrium conditions of mass transfer are assumed and no temperature dependency is taken into account.

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Two-Phase Flow Modeling in Porous Media Accounting for Fluid-Fluid Interfaces

Authors: Jennifer Niessner, Majid Hassanizadeh

We present a new numerical model for macro-scale two-phase flow in porous media which is based on a physically consistent theory of multi-phase flow. The standard approach for modeling the flow of two fluid phases in a porous medium consists of a continuity equation for each phase, an extended form of Darcy\'s law as well as constitutive relationships for relative permeability and capillary pressure. This approach is known to have a number of important shortcomings and, in particular, it does not account for the presence and role of fluid - fluid interfaces. The alternative is to use an extended model which is founded on thermodynamic principles and is physically consistent. In addition to the standard equations, the model uses a balance equation for specific interfacial area. The constitutive relationship for capillary pressure involves not only saturation, but also specific interfacial area. We present results of a numerical modeling study based on this extended model. We show that the extended model can capture additional physical processes compared to the standard model, such as hysteresis, and we demonstrate that results of the standard model can be fitted to that of the extended model by modifying relative permeability functions.

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Two-scale pore network modeling

Authors: Masa Prodanovic, Adrian P. Sheppard

Modeling multi-phase fluid flow in the subsurface is a notoriously difficult challenge. One must account for processes occurring on a broad range of scales; in particular the micro structure of the pore space frequently plays a critical role in determining macroscopic flow properties. To make things worse, different modeling approaches are demanded by the different length scales. Direct simulation in a detailed medium geometry is very costly. Modeling at the pore scale is thus normally done by mapping the pore space onto a representative network of idealized pores and throats and then modeling fluid displacements as discrete events on the pore-throat network. At larger scales, one usually constructs continuum numerical models in which individual grid blocks contain sufficiently many pores that the system within each grid block evolves smoothly with time. Continuum models capable of accounting for two scales - the so-called dual porosity models – have been constructed, and some efforts have also been made to build hybrid models. To our knowledge, all such efforts to bridge length scales have been done with at least one of the scales being continuum. While this is a natural consequence of experimental measurements where a single data point refers to a single length scale, with contributions from smaller scales averaged, there is nonetheless a loss of sub-scale features that might be relevant to the flow. Further, in most cases boundaries between the two scales must be simple, typically planar, a highly unrealistic simplification for the vast majority of porous materials. As described below, we propose to overcome these issues with pore network models. Pore space characterization on a wide range of scales is now becoming available, albeit from disparate sources. X-ray micro-computed tomography is nowadays widely used for imaging rock cores and granular packings; a single image can capture features ranging in size from several microns to one or two millimeters, while larger features can also be probed using this technology. One can identify the relevant length scales in a particular sample through nuclear magnetic resonance, mercury intrusion and adsorption isotherm experiments. Additionally, process-based and statistical reconstruction techniques are now being used by several groups to build three-dimensional pore space reconstructions on the submicron scale from electron micrographs. Unfortunately, these approaches are very computationally intensive and are therefore limited to studying very small volumes. Recently, focused ion beam tomography has been employed to give true three-dimensional images of similarly small volumes of carbonate rocks with nanometer resolution. It would be of great interest to directly utilize experimental information from more than one source in flow modeling. One can think of a representative pore-network as an extremely compact distillation of the original space down to only those parameters that matter for multiphase flow. The compactness of the representation enables one to capture more length scales than is possible with an image. We therefore propose to construct large pore-throat networks that incorporate data from two different imaging modalities at different length scales. In these networks the boundary between the length scales can take an arbitrary shape. We present an algorithm to geometrically match pore throat networks from two separate scales, that can be extracted directly from three-dimensional images, or be constructed to match the relevant small-scale properties of the pore space. Since the resultant pore network is a single entity, we can apply existing network modeling techniques, without requiring any additional \"bridging physics\" to stitch the length scales together. We present preliminary results from application of these network models.

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Uncertainty assessment of subsurface solute transport by transmissivity conditioning in finite heterogeneous domains

Authors: Giovanna Darvini, Paolo Salandin

Dealing with transport analysis in naturally heterogeneous porous aquifers, in the unconditional stochastic approach actual measurements may be used to infer the statistics of the formation hydraulic properties (e.g. porosity, transmissivity, storativity, etc.), and to give an estimation of the solute cloud evolution in terms of low order spatial moments. Nevertheless these moments reflect the mean transport characteristics in an imaginary medium of given statistical properties that may look different from the real case, that is the single realization observed. In the real case finite domain, the uncertainties in the flow and solute transport estimates may be reduced by properly accounting for the effects due to the boundary, and by conditioning the solution of the problem on available measurements of the hydraulic conductivity and/or potential head. Both the conditioning procedure and the boundary constraint affect the velocity statistics, whose statistical moments become dependent on its spatial position, so that the flow field statistical homogeneity cannot be invoked yet. In the paper the effect of the transmissivity conditioning on the flow field and on the inert solute plume evolution is investigated in finite 2-D domains by the stochastic finite element method (SFEM). This approach is able to handle any combination of finite complex boundary domain, medium nonstationary features, such as layers and geologic structures, by accounting for realistic flow configurations, as an example, due to the pumping and injecting wells. The only limitation being related to the log transmissivity variance of the media that must be small (less than unity) to theoretically ensure the validity of this perturbative approach. To evaluate the performance of the proposed solution, a synthetic heterogeneous 2-D aquifer is simulated by assigning at each square element of the computational grid the proper log transmissivity value obtained from a single unconditional realization. The field, conditioned on some of these like measured values extracted from the synthetic aquifer, is generated by use of the SGSIM code and the inhomogeneous flow field is achieved by SFEM. Therefore the flow nonstationarity due to the effect of boundaries is also felt. The velocity field covariance matrices allow to obtain the spatial moments of a solute plume by a first order Lagrangian analysis. The results obtained in the case of high Peclet values, that is by neglecting the pore scale dispersion, are compared in terms of velocity and particle displacement statistics with those achieved via Monte Carlo simulations expressly developed. The compared results give a measure of the performance of the proposed approach and demonstrate its ability to reduce the uncertainty in the solute plume evolution by conditioning.

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Understanding the interplay of increased pressure, residual heat and geologic and geochemical environment on radionuclide migration from underground nuclear tests

Authors: Reed M Maxwell, Russell L Detwiler, Qinhong Hu, Andrew FB Tompson

Understanding the processes that govern migration of radionuclides from underground nuclear tests is a problem of interest in many places in the world. Whether to gain understanding in the risks to human health, to guide water resources management decisions or as a surrogate for nuclear repository safety, there are a number of complex, coupled processes governing fate and form of radionuclides in the subsurface that need to be understood. These processes include the increased pore water pressure that is present after some underground nuclear tests, the residual heat signature from the nuclear detonation and the natural (i.e. pre-test) and altered (i.e. post-test) hydrogeologic and geochemical setting. We will focus on tests in saturated and unsaturated environments in Yucca Flat at the US Nevada Test Site. These tests all encompass a range of the aforementioned process interactions and provide insight into the broader context of understanding radionuclide migration from underground nuclear tests over a range of scale and environment. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This work was performed in support of the National Nuclear Security Administration, Department of Energy, Nevada Site Office, Underground Test Area Project.

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Understanding watershed processes and feedbacks using a fully-coupled groundwater, land-surface, surface water and mesoscale atmospheric model.

Authors: Reed M Maxwell, Fotini K. Chow, Stefan J Kollet

A variably-saturated groundwater flow model coupled with an integrated overland flow component, a land-surface model and a mesoscale atmospheric model is used to examine the interplay between coupled water and energy processes. These processes are influenced by land-surface topography and subsurface heterogeneity. This parallel, integrated model simulates spatial variations in land-surface forcing driven by three-dimensional atmospheric and subsurface components. Spatial ad temporal statistics are used to demonstrate correlations between land surface and lower atmospheric variables and water table depth. These correlations are particularly strong during times when the land surface temperatures trigger shifts in wind behavior, such as during early morning surface heating. A number of case studies are explored using this model. Regional-scale synoptic simulations forced from larger, nested models are used to diagnose land surface feedbacks on frontal systems and local rainfall distribution. Additionally, simulations of watershed response, runoff, groundwater and atmospheric feedbacks for a range of future climate conditions are presented. These simulations all point to the need to model the terrestrial hydrologic cycle as one system and to understand the interplay between the numerous coupled processes of which it is composed. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Upscaling Nonpoint Source Pollution with Nitrate: A Regional Modeling Approach

Authors: Thomas Harter, Andrea Cortis, Martin VanderSchans

Nitrate contamination is due to numerous sources including aerial deposition, septic systems, animal agriculture, fertilizer applications, and land application of urban/industrial wastes. We introduce a framework for statistical risk analysis of regional groundwater nonpoint source pollution in production wells that is based on numerical upscaling of local and field-scale processes to the regional scale; we present an efficient numerical procedure for its implementation; and validate the approach using a case study in the northern San Joaquin Valley dairy region. Our principal hypothesis is that regional variability of and uncertainty about well pollution from nonpoint sources is primarily caused by the spatio-temporal variability of the nonpoint source strength (recharge rate and recharge pollutant concentration) and the variable spatial distribution of pumping wells, pumping rates, and other groundwater discharge relative to the location of the nonpoint sources. Hence, the flow and transport equations are effectively subject to random forcing in the nonpoint source and pumping boundary conditions (external variability). The random forcing analysis yields a transient probability distribution function of water quality (water quality pdf) in a regional set of quasi-randomly distributed, discrete production wells and other groundwater discharge areas. The approach is implemented through a Matlab/Comsol based groundwater flow and transport code that ties into ArcGIS for generation of the quasi-random source and sink boundary conditions. Test-applications of this approach to an agricultural area show that the approach accurately captures the regional nitrate contamination trend and explains more than 70% of the variability in nitrate concentration between domestic wells.

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Use of Coupled Hydrological-Geophysical Modeling Framework for Exploring the Impact of Recharge on TDS

Authors: Michael B. Kowalsky, Stefan Finsterle, David B. Watson, Susan S. Hubbard

Time-lapse electrical resistance tomography (ERT) data, used in conjunction with wellbore data, have the potential to illuminate the spatiotemporal dynamics of infiltration and the associated variations in total dissolved solids (TDS) due to dilution via recharge. The overall objective of this work is to use such data, incorporated in a coupled hydrological-geophysical modeling framework, to obtain insight into the subsurface processes associated with natural episodic, seasonal, and annual recharge at the DOE Oak Ridge Integrated Field Challenge site. The modeling framework that we have developed for this purpose allows us 1) to systematically incorporate disparate datasets (hydrological, geophysical, and geochemical) and explore their sensitivities to variations in lithology versus TDS; 2) to investigate the temporal lag between high recharge events and subsurface TDS responses; and 3) to gain insight at the local scale which can then be transferred to the site-wide modeling effort using sparser but more spatially extensive datasets (such as surface ERT data). The potential of the approach will be demonstrated using a local-scale coupled hydrological-geophysical model of the drainage ditch near the S-3 pond at the site. The synthetic study is based on the planned experimental design and expected site conditions, and includes the following components: 1) construct 2-D model domain representative of the subsurface (vadose and saturated section) based on nearby wellbore data; 2) adjust model so that infiltration characteristics are adequately captured, based on available rainfall, pressure, water content, and temperature; 3) construct coupled hydrological-geophysical model that includes petrophysical relationship accounting for changes in ERT response due to changes in water saturation distribution in the vadose zone and TDS variations in the saturated zone; 4) test the joint inversion methodology for estimating hydrological parameter distributions and changes in hydrogeochemical properties over time. This study will allow us to evaluate the sensitivity of the various data types considered in the project for estimating the hydrological parameters of interest and evaluating the sensitivity of the ERT datasets in the saturated zone to freshwater recharge and associated dilution effects. The insight gained in this study will be useful for guiding the ongoing site-wide effort, which aims at understanding the influence of recharge on contaminant concentrations and natural attenuation mechanisms. Future work will consider the incorporation of surface-based geophysical data (e.g., surface ERT and self potential or SP) and isotopic data into the approach. This work was supported by the U.S. Dept. of Energy under Contract No. DE-AC02-05CH11231.

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Using a weather analogy to understand how to communicate ground-water model uncertainty

Authors: Mary C Hill, Eileen P. Poeter, Laura Foglia

Groundwater systems tend to be data poor and slow moving; weather systems tend to be relatively data-rich and fast moving. Ground-water modelers struggle to have their model predictions used to make policy decisions; weather forecasters have their predictions used routinely for day-to-day policy decisions. Groundwater modelers and their customers refrain from providing and asking for measures of uncertainty because, they say, it would make the models lose credibility; weather predictions without an analysis of uncertainty are thought to be less credible. What is happening here? This talk explores the difference in how system variability and model uncertainty are perceived in predictions from weather and ground-water models. The importance of analogous, extensively measured groundwater systems and site-specific, data-constrained simulations are considered. The importance of accounting for data error, the utility of sensitivity analysis and uncertainty quantification methods based on local and global methods, the consideration of alternative models, and other aspects of relating models and data are discussed. It is suggested that making ground-water models more useful by developing standard methods of communicating predictions and their uncertainty is critical to the future of ground-water engineering and science. The methods discussed are accessible through, for example, the computer codes UCODE_2005, OPR-PPR, and MMA, all of which are constructed using the JUPITER API.

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Using Ensemble Kalman Filter to Simulate Groundwater Flow and Solute Transport in Heterogeneous Media with Unknown Contamination Sources

Authors: Bill X. Hu, Chunlin Huang, Xin Li, Ming Ye

Hydraulic conductivity distribution and plume initial source are two important factors to affect solute transport in a naturally heterogeneous medium. Due to economic and technologic limitations, hydraulic conductivity can only be measured at limited locations in a field. Therefore, its spatial distribution in a complex heterogeneous medium is generally uncertain. In many groundwater contamination sites, solute initial conditions are generally unknown. The plume distributions are available only at sometimes after the contaminations occurred. In this study, a data assimilation method is developed for calibrating a hydraulic conductivity field and improving solute transport prediction with unknown initial condition. Ensemble Kalman filter (EnKF) is used to update the model parameter (i.e., hydraulic conductivity) and state variables (i.e., hydraulic head and solute concentration), when data are available. Two-dimensional numerical experiments are designed to assess the performance of the EnKF method on data assimilation for solute transport prediction. The study results indicate that the EnKF method will significantly improve the estimation of the hydraulic conductivity distribution and solute transport prediction by assimilating hydraulic head measurements with a known solute initial condition. When solute source is unknown, solute prediction by assimilating continuous measurements of solute concentration at a few points in the plume will well capture the plume evolution process in downstream.

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Validating the Multiscale Thermohydrologic Model Using an Alternative Model of the Proposed Repository at Yucca Mountain

Authors: Yue Hao, Thomas A. Buscheck, Yunwei Sun, Souheil Ezzedine, Scott C. James

The MultiScale ThermoHydrologic Model (MSTHM) is used in the total system performance assessment (TSPA) for the proposed nuclear-waste repository at Yucca Mountain. The MSTHM uses the Nonisothermal Unsaturated Flow and Transport (NUFT) code to represent thermal-hydrologic (TH) processes occurring at scales from a few tens of centimeters around individual waste packages and emplacement drifts (tunnels) all the way to the kilometer scale for heat flow through the mountain. The MSTHM is computationally more efficient than a monolithic 3-D TH model because it breaks the problem into smaller tractable pieces. An MSTHM simulation is constructed with NUFT-submodel calculations of various levels of coupled-process detail and scale, by superposing results of 3-D mountain- and drift-scale thermal submodels onto those of 2-D drift-scale TH submodels. The MSTHM was previously validated against an alternative (monolithic) 3-D TH model for a test problem at a scale smaller than the Yucca Mountain repository. Good agreement with the alternative model was obtained for temperature, relative humidity, and liquid saturation. A parallel-CPU version of NUFT handles much larger and more computationally demanding problems. This version is applied to an alternative (monolithic) 3-D "pillar-scale" TH model to simulate near-field and in-drift TH behavior along a full-scale (~1000-m long) emplacement drift. Results from the alternative model are compared to corresponding MSTHM results. Agreement with the alternative model builds confidence in the MSTHM applied at the scale of the Yucca Mountain repository. This study justifies key assumptions used in the MSTHM, such as that of negligible vapor flow along emplacement drifts. The pillar-scale model is also used to conduct a sensitivity study of parameters that control the magnitude of vapor flow and condensation along emplacement drifts. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract No. DE-AC52-07NA27344. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Validating Thermohydrologic Models Using the Drift Scale Test of the Proposed Repository at Yucca Mountain: Impact of Capillary-Pressure Cap

Authors: Yunwei Sun, Kenrick Lee, Thomas A. Buscheck, Scott C. James, Yue Hao

The MultiScale ThermoHydrologic Model (MSTHM) supports the total system performance assessment (TSPA) for the proposed nuclear-waste repository at Yucca Mountain. The MSTHM uses the Nonisothermal Unsaturated Flow and Transport (NUFT) code to represent thermal-hydrologic (TH) processes occurring at scales from a few tens of centimeters around individual waste packages and emplacement drifts (tunnels) all the way to the kilometer scale for heat flow through the mountain. The TH model involves two-phase (liquid and gas) nonisothermal flow and transport in an unsaturated fractured rock system, using a dual-permeability model of overlapping fracture and matrix continua. The TH model depends on calibrated system parameters, including the van Genuchten α and m parameters for the capillary pressure versus saturation relationship. Waste-package heat generation can drive liquid saturation to below residual saturation. Extending the van Genuchten capillary-pressure function to below residual saturation involves establishing a physically reasonable capillary-pressure cap. Various extension methods are considered for the van Genuchten capillary-pressure function as applied to a 3-D nested-mesh TH model of the Drift Scale Test (DST), as well as a corresponding 2-D drift-scale TH submodel, which supports the MSTHM. Simulated temperatures and liquid saturations are compared with field measurements from the DST. Compared to past DST model-validation studies, agreement between the simulated results and field measurements is improved, partially due to implementing a capillary-pressure cap. Because the same hydrologic properties and capillary-pressure cap are applied in the TH submodels supporting the MSTHM, this model-validation study builds confidence in the MSTHM as it is applied to Yucca Mountain TSPA. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract No. DE-AC52-07NA27344. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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MODELLING AND SIMULATIONS OF THE CHEMO-MECHANICAL BEHAVIOUR OF LEACHED CEMENT-BASED MATERIALS.

E. Stora1,2,*, B. Bary1, Q.-C. He2, E. Deville3, P. Montarnal3

1Atomic Energy Commission, CEA Saclay DEN/DANS/DPC/SCCME/Laboratoire d'Etude du Comportement des Bétons et des Argiles, 91191 Gif sur Yvette, France.

2Université Paris-Est, Laboratoire de Modélisation et Simulation Multiéchelle,

FRE3160 CNRS, 5 boulevard Descartes, 77454 Marne-la-Vallée Cedex 2, France

3CEA Saclay DEN/DANS/DM2S/SFME/MTMS, 91191 Gif sur Yvette, France.

The service life of cement-based materials, which can be employed in underground structures for nuclear waste disposal, is affected by different deterioration factors, such as chemical attacks and mechanical damage. Two particular sources of degradation that may interact with each other and have detrimental consequences on concrete underground facilities are presently focused on: (i) dissolution – precipitation reactions caused by ionic migration, governed by the material transport properties, between the interstitial solution and ground water; (ii) damage due to external mechanical loadings. Our objective consists in investigating the long-term behaviour of cementitious materials by simulating their response to these combined chemical and mechanical solicitations.

The French Atomic Energy Commission (CEA) has developed a numerical integration platform ALLIANCES that combines a speciation code (CHESS) and a finite volume/element code (CAST3M). This platform thus allows for simulating problems that couple chemistry, transport and mechanics and for predicting the chemo-mechanical degradations of structures made of mortar or concrete. The resistance of cement-based materials to these deteriorations is yet strongly conditioned by their mechanical and diffusive macroscopic properties. For this purpose, a multi-scale homogenization approach and a micromechanical orthotropic damage model are developed and implemented into the ALLIANCES platform to accurately estimate the evolutions of the material effective properties. Simulations of the chemo-mechanical behaviour of leached cementitious materials are carried out with the tool thus obtained and confronted with available experiments on mortar beams. The numerical results provide valuable information in terms of the material durability and in particular evidence a strong impact of the chemical alteration of mortar due to leaching on its overall mechanical behaviour.

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Virtual Globes as Tools of Hydrologic Data Discovery and Visualization

Authors: Bora Beran, Catharine van Ingen, Tom Barclay

Web mapping tools have significantly simplified the access to high quality imagery and maps without need to locally installed GIS software. However these tools offer maps for general consumer use (such as road networks, political boundaries and businesses) limiting their usefulness in the area of science. We've been developing tools to further the capability of these mapping environments with GIS functionality supporting vector/raster operations and additional data layers such as hydrography, geology and aquifers of the US. Exploiting the geographical relationships between elements of these data layers introduces a number of new paths for discovery of data published by various national agencies as well as individual researchers.

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Vortex methods and cavitation

Authors: Leonardo Traversoni

We present a modified vortex method using a hypercomplex representation of vortex transport equation. It has been observed that vortices are at the start of the formation of cavitation bubbles and at the final implosion of them. Using this method we can consider the bubbles as a singularity formed by high energy very local vortices and then predict without costly laboratory experiments the behaviour of the cloud of bubbles. Also the inherent energy of them may be obtained in ordet to predict its destructive effects in species mixed with the cavitating fluid.

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Water Supply Systems in Groundwater/Surface-water Models

Authors: Sorab Panday, Terry Foreman, Vivek Bedekar, Nate Brown, Prasanna Sampath, Jagjit Kaur

Extraction of groundwater is an example of a specified boundary condition in groundwater flow models. Likewise, irrigation application and urban discharge to streams are examples of specified boundary conditions in surface water flow models. However, these water components are often interrelated in groundwater/surface-water models because the extracted groundwater might be routed and reapplied within the physical system via irrigation or water treatment plant discharges. When the irrigated land use changes through time or when water quality of the source water are important components of a modeling study, implementation of linked boundary conditions is an important consideration in terms of quantifying applied water quantity and quality. For example, future water quality of extracted groundwater is typically not known a priori for a given water supply projection; however, the quality of this extracted groundwater could be important for projections of water quality of irrigation water, discharges from water treatment plants, and resulting water quality distributed throughout a modeling domain. These issues can be resolved by use of a Water Supply System (WSS), which assimilates sources of water supply in terms of water quantity and quality through time and dynamically distributes this water for indoor and outdoor use within the WSS service area within the model domain. Irrigation water is applied to the land surface according to land use distributions which can vary through time and in proportion to water demand of each land use type which can further vary seasonally. Water used indoors can be injected into the subsurface, reapplied on the land surface, discharged to streams, or removed from the model domain. In addition, a WSS may also add or remove solute mass to or from the water before reapplication or discharge to streams to simulate loading or removal of a given solute. The concept and formulation of a WSS within the context of a groundwater/surface-water model are discussed, and an application example is provided to demonstrate its use and utility.

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