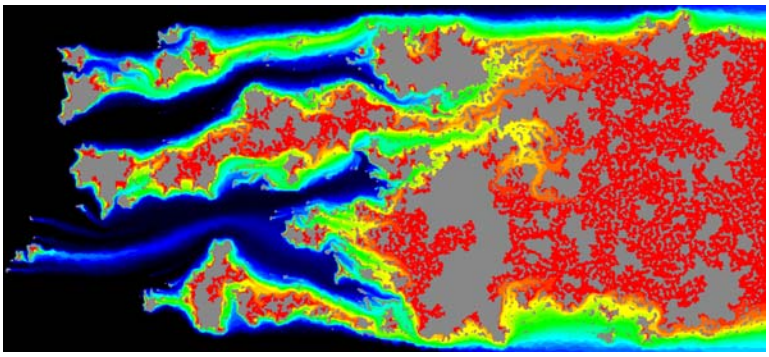
Flow and Transport: Characterization and Modeling from Pore to Reservoir Scales



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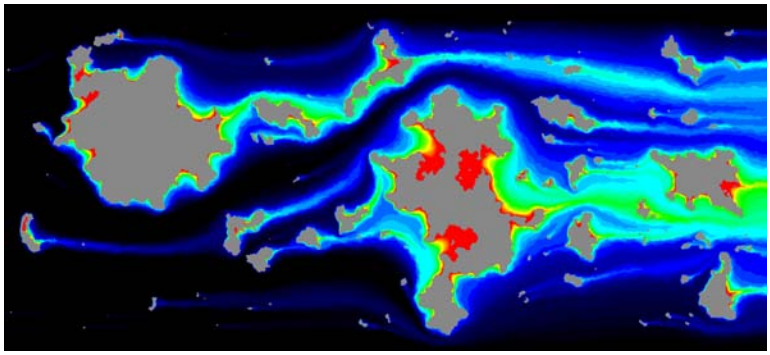

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Figure from Robert Glass

Gaithersburg Marriott Washingtonian Center
Gaithersburg, MD
September 24-25, 2004

FORWARD

"Flow and Transport: Characterization and Modeling from Pore to Reservoir Scales" is the eleventh in a series of Geosciences Research Program Symposia dating from 1995. These symposia are topically focused meetings for principal investigators in the program and provide opportunities for our investigators to give presentations to one another and to discuss their Office of Basic Energy Sciences' supported research. In addition to the recognition the symposium gives to all of the investigators, we traditionally also recognize one outstanding contribution from a DOE Laboratory Project and one from a University Project. The outstanding contributions are selected by our session chairpersons. We are fortunate to have as guest session co-chairs Professor Roger Beckie from the University of British Columbia, Professor Ronald Falta from Clemson University, Professor Mario Ioannidis from the University of Waterloo, and Dr. Michael J. King from BP. They join our Principal Investigator co-chairs Professor Katherine McCall of the University of Nevada, Professor Amos Nur of Stanford University, Dr. Karsten Pruess of the Lawrence Berkeley National Laboratory, Dr. Wenlu Zhu of the Woods Hole Oceanographic Institution. For their efforts on behalf of the investigators I thank them all. We are looking forward to an outstanding series of presentations.

Nicholas B. Woodward
Geosciences Research Program
Office of Basic Energy Sciences
U.S. Department of Energy

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Gaithersburg, MD
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9:20 Christopher M. Reddy, Woods Hole Oceanographic Institution
2DGC- A New Window on Subsurface Oil and Gas Migration

9:45 Mack Kennedy, Lawrence Berkeley National Laboratory
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10:40 Edward Bolton, Yale University
Models of Kinetically Controlled Fluid/Rock Interaction in Earth's Crust

11:05 Jonathan Price, Rensselaer Polytechnic Institute
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11:30 Wenlu Zhu, Woods Hole Oceanographic Institution
Evolution of Pore Structure and Permeability of Rocks under Hydrothermal Conditions

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7:00 **Banquet**

Reactive Transport Modeling of Hydrocarbon Migration, Fluid Mixing and Fault Mineralization, Santa Barbara Basin, California

Grant Garven

Department of Earth & Planetary Sciences, Johns Hopkins University, Baltimore, MD 21218

The Santa Barbara basin is a 100 km-long trough originating from transpression of the southern California continental margin beginning in the late Oligocene. The basin has been a prolific source of hydrocarbons that occur in at least 70 distinct fields in Cretaceous to Holocene sediments, with the greatest concentrations occurring in Neogene sediments. Uplift of the northern margin of the basin beginning in the Pliocene created a broad zone of meteoric recharge in the Santa Ynez Mountains and several prominent east-west trending faults such as the Refugio-Carneros fault (Figure 1). Extensive calcite cements containing isotopically light carbon ($\delta^{13}C$ = -30 to -40‰) and high fluid inclusion homogenization temperatures (85-100º C) found along some of the shallower portions of the Refugio-Carneros fault indicate that the faults may have been the foci of mixing between oxidizing meteoric water and methane-rich basinal fluids. Numerical reactive transport models of a structurally complex and geologically heterogeneous 2-D profile across the basin support this hypothesis. In the models, oxidizing meteoric water enters steeply dipping aquifers outcropping in the Santa Ynez Mountains, displacing methane-bearing formational fluids and producing weak calcite mineralization along the mixing front. The greatest concentrations of calcite are precipitated in the upper levels of the Refugio-Carneros fault due to the higher magnitude and duration of methane flux in the fault as a result of its high permeability and intersection of multiple methane-rich strata. Faults were also shown to be important conduits for heat transport. The high heat flow in the basin and rapid ascent velocities driven by buoyancy and overpressuring allow model temperatures in the Refugio-Carneros fault to exceed fluid inclusion homogenization temperatures at depths within 100 meters of the ground surface, further contributing to calcite mineralization by locally increasing temperature.

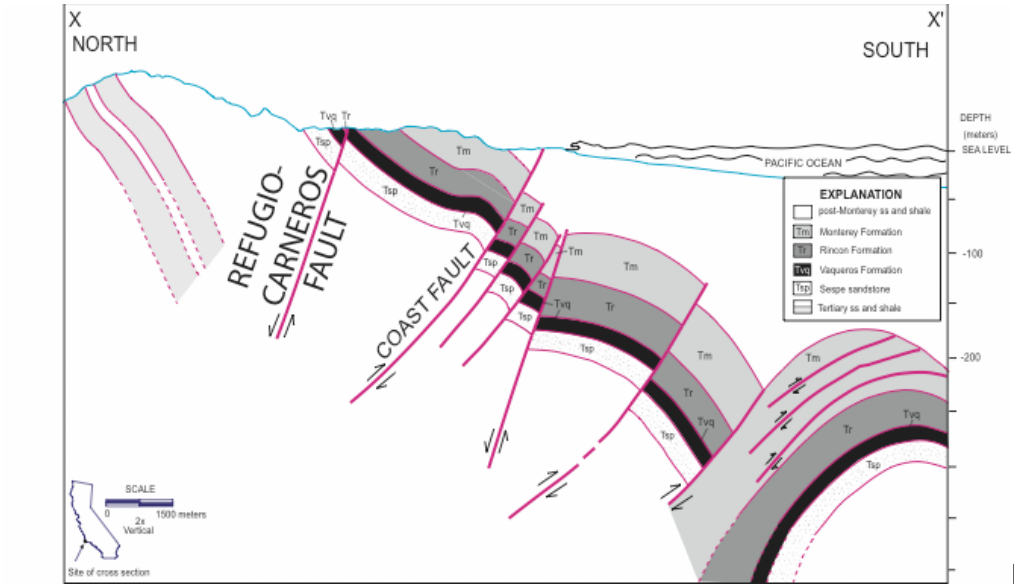

Figure 1

Understanding Long-term Solute Transport in Sedimentary Basins: Simulating Brine Migration in the Alberta Basin, Canada

Alicia Wilson

Department of Geological Sciences, University of South Carolina, Columbia, SC 29205

Knowledge of large-scale solute transport in sedimentary basins is critical for understanding petroleum migration, formation of ore deposits, and chemical diagenesis of sediments, but solute transport in such settings remains poorly understood. In particular, geochemical and hydrogeologic estimates of the residence time of fluids in sedimentary basins contrast strongly. Geochemical studies of brines have suggested that ancient evaporatively-concentrated brines have been preserved in sedimentary basins for hundreds of millions of years, but hydrogeologic studies have emphasized the difficulty of preserving brines and large salinity gradients over long periods. This project was designed to address this apparent conflict by using geochemical data to constrain advanced numerical models of brine migration during the evolution of the Alberta Basin, Canada. Simulations of variable-density fluid flow, sediment compaction, heat transport, solute transport, dissolution of evaporites, and groundwater age are in the early stages of development and are designed to generate quantitative estimates of porefluid residence times in the Alberta Basin.

Previous hydrogeologic simulations of brine flushing may have over-estimated the permeability of deep sedimentary rocks, thereby over-estimating the rate of topography-driven flushing of brines. The low permeability of thick shales in the Alberta Basin has undoubtedly played a role in the preservation of deep brines, but current work suggests that abnormal pressures in these beds could also have created a hydrodynamic barrier to solute transport. Low permeabilities limit advective and dispersive transport, but local flow patterns associated with abnormally-pressured beds have the potential to limit diffusion as well, which may be significant for preserving ancient brines. Large salinity gradients in the Alberta Basin also suggest that density gradients could have affected the depth of topography-driven flushing. Finally, foreland basins of similar history but further south in the US mid-continent region provide a useful contrast to the Alberta Basin. In the midcontinent region, brines are apparently derived from dissolution of evaporites rather than preservation of ancient evaporatively-concentrated fluids. This difference suggests a shorter fluid residence time in the midcontinent than in the Alberta Basin. New estimates of residence time in these systems will be important for understanding the origin and migration of brines, sedimentary diagenesis, and, potentially, the suitability of these systems for carbon sequestration.

Analyzing Complex Mixtures of Petroleum Hydrocarbons in the Surface and Subsurface With Comprehensive Two-Dimensional Gas Chromatography (GC×GC)

Christopher M. Reddy, Lorraine B. Eglinton, Robert K. Nelson, and Jean K. Whelan

Department of Marine Chemistry and Geochemistry, Woods Hole Oceanographic Institution, Woods Hole, MA 02543

One of the most promising new techniques for analyzing complex mixtures of petroleum hydrocarbons in the surface and subsurface is comprehensive two-dimensional gas chromatography (GC×GC). This technology is capable of separating an order of magnitude more components in hydrocarbon mixtures than traditional gas chromatography, which is generally limited to mixtures containing fewer than one hundred components. This increased resolution is achieved by using two chromatographic columns with different stationary phases coupled together by a modulator that transfers all of the analytes from the first column to the second column. The modulator uses alternating jets of hot and cold gas to modulate analytes. GC×GC is significantly different than more typical "heart-cutting" two-dimensional gas chromatography, which only allows select components from the first column to be chromatographically separated on a second column. In GC×GC, there is complete mass transfer from the first column to the second column and therefore the technique is comprehensive. In addition to the dramatic improvement in resolution that GC×GC enjoys over traditional one- or even traditional two-dimensional gas chromatography, this approach also yields increases in sensitivity. This is because of the focusing effect of the modulator, and the small dimensions of the second column, which together result in very narrow, sharp peaks, typically on the order of 100-250 ms wide. The accompanying increase in signal-to-noise corresponds to order of magnitude increases in sensitivity. Perhaps, the most important attribute of GC×GC to understanding flow and transport of petroleum is the "chemical ordering" in which compounds in the same class elute along the same plane. The three-dimensional data arrays generated by GC×GC are also ideally suited for producing difference chromatograms, which can identify subtle differences in discrete samples. Examples of this technology and future efforts will be discussed.

Diffusive Separation of Noble Gases and Noble Gas Abundance Patterns in Sedimentary Rocks

T. Torgersen[1], B.M. Kennedy[2] and M. C. van Soest[2]

[1]*Department of Marine Sciences, University of Connecticut, Groton, CT 06340*
[2]*Center for Isotope Geochemistry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720*

The mechanisms responsible for noble gas concentrations, abundance patterns, and strong retentivity in sedimentary lithologies remain poorly explained. Diffusion-controlled fractionation of noble gases is modeled and examined as an explanation for the absolute and relative abundances of noble gases observed in sediments. Since the physical properties of the noble gases are strong functions of atomic mass, the individual diffusion coefficients, adsorption coefficients and atomic radii combine to impede heavy noble gas (Xe) diffusion relative to light noble gas (Ne) diffusion. Filling of lithic grains/half-spaces by diffusive processes thus produces Ne enrichments in the early and middle stages of the process with F(Ne) values similar to that observed in volcanic glasses. Emptying lithic grains/half-spaces produces a Xe-enriched residual in the late (but not final) stages of the process producing F(Xe) values similar to that observed in shales. 'Exotic …but unexceptional' shales that exhibit both F(Ne) and F(Xe) enrichments can be produced by incomplete emptying followed by incomplete filling. This mechanism is consistent with literature reported noble gas abundance patterns but may still require a separate mechanism for strong retention. A system of labyrinths-with-constrictions and/or C-, Si-nanotubes when combined with simple adsorption can result in stronger diffusive separation and non-steady-state enrichments that persist for longer times. Enhanced adsorption to multiple C atoms inside C-nanotubes as well as dangling functional groups closing the ends of nanotubes can provide potential mechanisms for 'strong retention'. We need new methods of examining noble gases in rocks to determine the role and function of angstrom-scale structures in both the diffusive enrichment process and the 'strong retention' process for noble gas abundances in terrestrial rocks.

Models of Kinetically Controlled Fluid/Rock Interaction in Earth's Crust

Edward W. Bolton, Danny M. Rye and Jay J. Ague

Department of Geology and Geophysics, Yale University, New Haven, CT 06520

Modeling, field, and laboratory studies are combined to elucidate the nature of fluid/rock interaction in Earth's crust over a broad range of temperature conditions. The modeling effort focuses on diffusion, as well as fluid flow and transport, with exchange via kinetically controlled mineral dissolution and precipitation reactions, as well as isotopic and trace element exchange. New field-based chemical and isotopic data provide a framework for testing our models of flow, reaction, and isotopic exchange.

In one study of near-surface low-temperature weathering, we focus on the oxygen diffusion into black shales. Oxidation of ancient organic matter and pyrite in shales serves as one of the primary controls on the long-term evolution of atmospheric oxygen levels. The model, which includes erosion, diffusion, and kinetic control of oxidation rates, predicts that most unearthed ancient organic matter would oxidize before reaching the surface. In a separate infiltration model, we test the influence of hypothesized 70^{o}C Archean temperatures on surface mineral abundances in a soil derived from a simple granite, and compare to results predicted for present day surface temperatures.

Models of flow and reaction in siliceous dolomites in contact metamorphic settings predict that kinetic control is vital for the understanding of temperature-composition (T-X) pathways. Upon heating, the CO_2 rich supercritical fluid generated by decarbonation reactions leads to unexpected T-X pathways including dramatic overstepping of "equilibrium curves". Sub-gridscale grain models help show how initial grain size of the siliceous dolomite can influence the flow regime, with either buoyancy-drive or reaction-drive being possible. The model predictions are reinforced by field-based studies of morphological variations in metamorphic garnets that indicate substantial deviations from chemical equilibrium during nucleation and growth.

Field and modeling studies of metacarbonate rocks show that crustal fluids mobilize a wide variety of elements, including Al and the rare earths. In these low-permeability rocks, lithologic contacts and fractures were primary flow conduits that supported enormous fluid fluxes, consistent with field-modeling results for the subduction complex on Tinos, Greece.

Isotopic and trace element diffusion in grains is modeled simultaneously with fluid flow and grain growth and dissolution. Such modeling shows important kinetic effects are possible, even in high-temperature environments, as the rate of exchange between grain interiors and their rims may be comparable to (or slower than) rates of dissolution and precipitation. Comparisons with batch and fractional melting approximations are underway. Both the isotope and the trace element models will be used to better understand results from field studies underway.

Oxygen and carbon isotopic data from shallow-crustal rocks of the Conasauga Group, Tennessee, illustrates that the flow regime is critically dependent on rock type. Detailed sampling of veins and adjacent wall rocks in limestones show that a fluid of constant C and O isotopic composition was introduced in the cracks and that exchange was limited to a few millimeters. The C and O isotopic values of carbonate veins and matrix carbonate from shale units near the limestone contact indicate that the fluids in both were the same as the fluids introduced in cracks in the limestone units. Isotopic values of carbonates in near the base of the shale unit indicate a fluid that was probably produced by dewatering of the shale and oxidation of organic C. The observed trend, of decreasing isotopic values over the entire 90 m of the shale unit, suggests communication and mixing of fluids occurred throughout the porosity of the shale.

Experimental Studies of Grain-Scale Permeability and Pore Geometry in Deep-Seated Fluid-Bearing Rocks

Price, J.D., Wark, D.A., Thomas, J.B., and Watson, E.B.

Department of Earth & Environmental Sciences, Rensselaer Polytechnic Institute, 110 8th St., Troy, NY, 12180

In fluid-bearing polycrystalline materials subjected to conditions promoting rapid kinetics, the shape of grain boundary pores is controlled by the interfacial energy of the pore-fluid with the grains and along grain boundaries. The intersection angle of pore-walls with grain boundaries reaches its lowest value when all energies are minimized (dihedral angle, θ). Previous numerical modeling detailed the relationship between the porosity (ϕ) and the permeability (k) of rocks of uniform grain (and pore) size as a function of θ. Investigations by the authors directly evaluated the permeability of more complicated materials and examined the nature of interfacial energy and pore geometry on synthetic rocks to further constrain the distribution and transport of fluid in grain-scale pores.

Permeametry of quartzite and marble with aqueous fluids synthesized at elevated temperature and pressure determined the permeability of grain-boundary pores and with a non-uniform grain size. Quartzites contained pores with an average θ of 41^o and $k = 270\phi/3$ for a normalized 1 mm grain size. Marbles contained pores with an average dihedral angle of 65^o and $k = 200(\phi-0.015)/3$. Further experiments of quartzite with a volumetrically minor (2-7%) fine-grained mineral showed that additional phases slightly increase k for a given ϕ, but reduced it slightly with their increased volume fraction. These experiments suggest that grain-scale permeability of many real rocks is well predicted by the ideal numerical model.

Further complications produce deviations from the ideal model. Permeametry of synthetic rocks revealed that faceting may diminish permeability. While pyroxene quartzite containing pores ~50% faceted yield the same k-ϕ relationship as the not extensively faceted pure quartzite (mentioned above), synthetic amphibolite with pores >90% faceted exhibit k greatly reduced for a given ϕ. Despite a low interfacial angle, the faceting disconnects the pores in a manner similar to the high θ synthetic marbles, such that $k = 189(\phi-0.04)/3$. This finding suggests that extensively faceted rocks are less permeable than those with lower degrees of faceting.

Electron microscopy on sections of synthetic rocks showed that the distribution of interconnected pore fluids varies between materials of different grain size or composition. Runs juxtaposing two quartzites of different grain size contained fluids preferentially distributed to the material with smaller grain size due to the constant curvature of the pore walls. Those coupling two different monomineralic materials contained more voluminous pores (by as much as a factor of 5) in the material with the lowest pore interfacial energy. Both suggest that given an interconnected pore structure, fluids will partition to rocks composed of grains of lower interfacial energy or smaller grain size.

Electron microscopy on sections of experiments revealed the distribution of grain-scale pores formed in a thermal gradient. Synthetic quartzites equilibrated under a temperature gradient produced channels parallel to the gradient, the likely result of preferential dissolution and precipitation in fluids in a corresponding SiO_2 solubility gradient. Such features could increase permeability in one direction in materials subjected to large temperature gradients, like those associated with contact metamorphism.

Additionally, atomic force microscopy of experiments revealed the pore morphology of fluids introduced along synthetic grain boundaries produced by juxtaposing oriented and polished grains under

elevated temperatures and pressures. Results showed in 3-D that the intersection angle and overall morphology of the pores is a function of grain lattice mismatch. This suggests that grain-scale networks may be modified with changes in grain orientation (rock fabric).

Collaborative Research: Evolution of Pore Structure and Permeability of Rocks under Hydrothermal Conditions

Brian Evans[1] and Wenlu Zhu[2]

[1]*Massachusetts Institute of Technology, Cambridge, MA 02139*
[2]*Woods Hole Oceanographic Institution, Woods Hole, MA 02536*

Both temporal and spatial variations of permeability are common in the Earth; such variations are driven by a diverse and complex set of processes including fracturing, diagenesis, cementation, brittle pore collapse, compaction owing to pressure solution or plastic flow, crack healing, crack sealing. Each mechanism will respond to a particular set of driving forces, including local non-hydrostatic stresses; reduction of interfacial energy; dissolution into under saturated liquids, precipitation from oversaturated fluids, or reactions between phases. To identify the dominant process, kinetics laws need to be developed for each mechanism. It is useful, heuristically, to separate the rate of change of permeability with time into two separate factors. One is the rate of change of permeability with change in porosity, which we call "efficiency"; the second is the rate of change of porosity with time, which might be abbreviated as "RCP". Our research program is designed to investigate these factors in laboratory-scale rock samples, under conditions of elevated temperature and pressure, and to develop insight into the kinetics laws appropriate for natural conditions.

Both factors are strongly influenced by the details of the physical processes that are responsible. Some processes are more efficient in changing permeability than others. For example, neo-mineralization and dilatant micro fracturing are capable of producing large changes in permeability with relatively small changes in total porosity, but compaction during creep is less efficient, provided that capillary forces are capable of maintaining steady-state interfacial angles. Melt migration in a typical mantle rock is another example of fluid flow in a porous medium. Because direct measurements of permeability in partially molten materials are difficult, it is often necessary to estimate permeability and the efficiency of permeability change using knowledge of the melt phase distribution at the grain-scale. We developed a 3D network model to calculate permeability as a function of melt fraction for a system with a distribution of dihedral angles. This approach allows us to link the topology of melt phases and the geometry of individual melt channels to the bulk physical properties. Using this approach, we can quantify the effects of grain-scale heterogeneities on melt transport by explicitly incorporating the distribution of melt (including dihedral angle, melt channel connectivity etc.) in the network models. In our model, each channel is treated as a prism with a length of the grain edges. The cross-sectional area of each prism is determined by a given dihedral angle and a melt fraction. By incorporating different dihedral angles into a network model, we are able to model permeability of partially molten rocks, taking the grain-scale heterogeneity of melt distribution into account. Our results show that the permeability of a heterogeneous system can be significantly smaller than the calculated permeability of an isotropic system with the same median dihedral angle.

We are also conducting experiments to understand the physics of processes that control the rate of change of porosity, and, in particular, to isolate the effect on the transport properties of such processes as solution-transfer, brittle fracturing, dislocation creep, or single parameters like roughness of the pore surface, connectivity of the pore space, or heterogeneity of the transmissivity. The work include studies of: 1) deformation and permeability reduction in fluid-filled quartz rocks, 2) porosity and permeability evolution in calcite rocks under triaxial loading, 3) the effect of multi-scale heterogeneities and pore-wall

roughness on permeability. For example, when samples of Sioux quartzite were inserted into a hydrothermal pressure vessel and heat-treated at temperatures of 300-500°C confining pressures of between 300MPa and 125MPa and fluid pressures from 125MPa to 250MPa, permeability was reduced by as much as three orders of magnitude. Reductions occur fastest at higher temperatures and higher effective pressures.

Publications and Meetings Papers Funded by this Grant (2003-4):

In press (indicates author not funded by this grant):*

Bernabé, Y., U. Mok, and B. Evans, A note on the oscillating flow method for measuring rock permeability, *Int. J. Rock Mechanics and Mining Sci., submitted* March, 2004.

Bernabé, Y., U. Mok, B. Evans and F.J. *Herrmann, Permeability and storativity of binary mixtures of high- and low-porosity materials, *J. Geophys. Res., submitted*, 2004.

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*Walsh, J. and W. Zhu, Sliding of a rough surface under oblique loading, *J. Geophys. Res.*, 109, B05208, doi: 10.1029/2004JB003027, 2004.

Zhu, W., P. *Baud and T.-f. *Wong, Dilatancy and post-yielding behavior in porous sandstones: A new loading path, in *12th Panamerican Conf. on Soil Mechanics and Geothecnical Eng., Vol. 1*, ed. P. J. Culligan, H. H. Einstein and A. J. Whittle, 2003.

Xiao, X.-h., W. Zhu, and B. Evans, Deformation mechanisms and failure modes in Solnhofen limestone, *in press,* in *12th Panamerican Conf. on Soil Mechanics and Geothecnical Eng., Vol. 1,* ed. P. J. Culligan, H. H. Einstein and A. J. Whittle, 2003.

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Bernabé, Y., U. Mok, and B. Evans, Permeability-porosity relationships in rocks subjected to various evolutionary processes, *Pure Appl. Geophysics, 160,* 937-960, 2003.

Streamline based Flow Simulation and Characterization of Naturally Fractured Reservoirs

Akhil Datta-Gupta[1] and Richard L. Gibson[2]

[1]Department of Petroleum Engineering, [2]Department of Geology and Geophysics, Texas A&M University, College Station, TX 77845

It is well recognized that fractures can serve as highly conductive flow paths and often lead to unexpected reservoir performance. Adequate characterization and assessment of fracture density, orientation and distribution are vital to optimal exploitation and management of fractured reservoirs. In particular, calibrating high resolution geologic models to production history is an important step in fractured reservoir characterization. Recently streamline-based flow simulation has shown great potential in this regard. The streamline-based generalized travel time inversion which is analogous to seismic tomography, has been used to develop efficient and robust methods for production data integration into high-resolution reservoir models. Several field applications have demonstrated the practical feasibility of the approach.

We extend the streamline-based production data integration technique to naturally fractured reservoirs. Describing fluid transport in fractured reservoirs poses additional challenge arising from the matrix-fracture interactions. We first generalize the streamline models to fractured reservoirs by treating the fracture and matrix as separate continua that are connected through a transfer function as in conventional dual-porosity simulators. Second, we analytically compute the sensitivities that define the relationship between the reservoir properties and the production response. The sensitivities are critical to any inverse modeling and using streamline models we can compute them efficiently using a single forward simulation. This makes our approach particularly well-suited for large-scale field applications. Finally, production data integration is carried out via generalized travel time inversion which is extremely robust and utilizes established and proven techniques from geophysical inverse theory.

We demonstrate the power and utility of our approach using realistic synthetic examples and also a field application in a fractured limestone formation. The fracture patterns are generated using a discrete fracture network model that utilizes seismic and field derived parameters to distribute fractures as objects. Next, grid block permeabilities are assigned based on a fracture intensity index. Starting from this *prior* model, we incorporate water-cut histories using the generalized travel time inversion. Our results indicate that the proposed method is able to reproduce the dominant fracture patterns both in the synthetic and field applications. However, the reservoir models are still missing parts of the fracture systems, motivating the use of seismic data to provide additional constraints. Finally, we will present preliminary seismic model results in the form of reflection coefficients and synthetic seismograms to demonstrate how AVO and other seismic measurements have the potential to enhance reservoir characterization in combination with production data.

Microbes, Mass Transport, and the Chemical Evolution of Groundwater

Robert Sanford, Matthew Kirk, Jungho Park, Qusheng Jin, George Roadcap and Craig Bethke

Department of Geology, University of Illinois at Urbana-Champaign, Urbana, IL 61801

Groundwater in many deep aquifers is chemically zoned along flow. To investigate how microbial communities influence the chemical evolution and thus the zonation of groundwater, a succession of wells along the flow path were sampled from the Middendorf aquifer, in the South Carolina coastal plain. Water from the well-studied aquifer contains dissolved oxygen at the recharge area and progressively passes through zones of microbially mediated iron-reduction, sulfate reduction and methanogenesis. These zones, however, do not necessarily represent discreet areas within which other types of microbial activity are excluded. For example, sulfate reducing bacteria are active in the iron reducing zone and influence the chemical evolution of the groundwater there. To characterize biogeochemical evolution in the aquifer, we monitored the chemical and microbiological features of groundwater collected from the wells. Although the chemical analysis support discreet chemical zonation representing the differentiation of predominant electron accepting processes along the flow path, a metabolic energy analysis indicates that both iron reduction and sulfate reduction are thermodynamically favorable just downgradient of the recharge area. The microbiological analysis also supports this, since the results show that the composition of microbial biomass suspended in the groundwater is not zoned along flow. Nearly identical bacterial communities capable of iron and sulfate reduction grew in cultures from most of the sites we sampled. Little variation is present, furthermore, in the composition of biomass filtered directly from the groundwater. These findings suggest that microbial activity may not be defined by discrete zones, but rather reflect a balance between metabolic activities (e.g., iron reduction and sulfate reduction). Analysis of the CO_2 production in the non-marine sediments suggests that availability of ferric iron and sulfate are not limiting activity, but the availability of carbon (i.e. acetate) from fermentation processes controls the rate of microbial metabolism and thus is the main driving force for biogeochemical evolution within the aquifer.

Numerical Modeling of CO_2 Disposal in Saline Aquifers

Karsten Pruess and Chin-Fu Tsang

Earth Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720

The purpose of our research is to develop a systematic, rational, and mechanistic understanding of the coupled processes that would be induced by injection of CO_2 into saline aquifers. This is being accomplished by means of conceptual, mathematical, and numerical models that are based on rigorous continuum theories of fluid dynamics, coupled with detailed rock fracture mechanics and chemical speciation and reaction path analyses. Our presentation will review recent progress in process modeling capabilities, and in understanding of the dynamical behavior of CO_2 disposal systems.

We have developed a capability for modeling multiphase flows of water and CO_2 that includes all possible fluid phase combinations (aqueous - liquid CO_2 - gaseous CO_2), as well as transitions between supercritical and subcritical conditions. Improvements were made in the accuracy of thermophysical property description, including partitioning of water and CO_2 between aqueous and CO_2-rich phases, dependence of aqueous phase density on dissolved CO_2 content, and treatment of gas mixtures (CO_2, H_2S, SO_x and NO_x). These modeling capabilities have been applied to the problem of CO_2 leakage from geologic disposal reservoirs along fracture zones and faults, an important objective being to determine whether it is at all possible for CO_2 to be discharged in a self-enhancing, eruptive manner. Our simulations provide evidence for strong cooling effects arising from the expansion of supercritical CO_2. Eventually sub-critical conditions are reached, where additional cooling may occur when liquid CO_2 boils into gas. CO_2 discharges may show quasi-periodic cycling due to an interplay between heat transfer and multiphase flow effects.

Strong heat transfer effects were also found in CO_2 injection wells, and have been analyzed in connection with a pilot test of CO_2 injection that is about to commence in the Frio formation near Houston, Texas. Other studies performed in preparation for this test include modeling of CO_2 migration in heterogeneous 3-D media, and design of noble gas tracer tests as a means for characterizing in situ phase conditions.

More fundamental studies have examined hydrodynamic instabilities and the possibility of fingering flow and bypassing as more viscous water is being displaced by less viscous CO_2.

Development of a reactive chemical transport code TOUGHREACT has been completed. The code is being released to the public through DOE's Energy Science and Technology Software Center (ESTSC). TOUGHREACT augments our multiphase code TOUGH2 with a comprehensive description of reactions between aqueous, gaseous, and mineral species. Recent applications include CO_2 disposal into sand-shale systems as are found in sedimentary formations near the Texas gulf coast, and studies of injection of sour gases that in addition to CO_2 contain H_2S and SO_2.

Geomechanical aspects of CO_2 sequestration have been studied using the TOUGH-FLAC simulator that couples TOUGH2 with the commercial rock mechanics code FLAC3D. A newly developed capability for analysis of fault slip and leakage has been tested on a system consisting of a CO_2 injection zone that is laterally bounded by two inclined sealing faults. CO_2 was injected at high pressure until slip was triggered along the two bounding faults and the amount and the extent of the fault slip were calculated. Material parameters and injection scenarios representing a realistic CO_2 injection

case were used, similar to those at the Frio test site in Texas. In parallel, the TOUGH-FLAC code is being tested by simulation of *in situ* experiments, and by code-to-code intercomparison. Additionally, basic studies have been performed to study different fundamental aspects related to underground injection of fluids.

Using Geophysical and Hydrological Data to Estimate Flow Properties

D. W. Vasco

Earth Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720

Currently, time-lapse geophysical data are used primarily for reservoir monitoring. That is, time-lapse observations are used to map changes in reservoir saturation and pressure. The next logical step is to use time-lapse data to characterize the reservoir: to infer reservoir permeability and porosity heterogeneity. Such time-lapse generated models of reservoir permeability will aid in oil and gas recovery, geothermal production, and environmental remediation. Currently, there have been very few attempts at formal reservoir characterization using time-lapse observations. By formal reservoir characterization, I mean some manner of inversion of the time-lapse field data for reservoir flow properties. Reservoir characterization based upon time-lapse geophysical data is hampered by computational difficulties. Typically, finding a reservoir model that is compatible with a set of saturation and pressure changes, as would be derived from the time-lapse data, requires a significant number of reservoir simulations. Because each reservoir simulation may take hours, if not days, of CPU time on a workstation, formal inversion can be prohibitively expensive. For example, stochastic methods, such as the simulated annealing approach, require hundreds, if not thousands of reservoir simulations.

Asymptotic methods provide an efficient means by which to infer reservoir flow properties, such as permeability, from time-lapse geophysical data. A trajectory-based methodology, similar to ray-based techniques for medical and seismic imaging, provides the foundation for an iterative inversion of time-lapse data. This approach requires a single reservoir simulation for each iteration of the algorithm. In this talk I describe the basic elements of the approach and illustrate it with applications to the inversion of time-lapse seismic observations. In effect, the time-lapse observations are used to constrain changes in saturation and pressure. Asymptotic expressions are then used to relate the saturation and pressure changes to reservoir flow properties. A perturbation approach is used to derive sensitivities, relating time-lapse seismic amplitude changes to flow property perturbations. A comparison between purely numerical and the trajectory-based sensitivities demonstrates their accuracy. Analysis of a set of synthetic amplitude changes indicates that one is able to recover large-scale reservoir permeability variations from time-lapse seismic amplitude data.

An application to actual time-lapse amplitude changes from a field in the Gulf of Mexico demonstrates that the approach is both practical and efficient. Time-lapse data were gathered over a producing field, spanning some eleven years of production. Using the trajectory-based technique, I am able to reduce the misfit to the time-lapse amplitude changes by 81% in twelve iterations. The resulting model indicates that lower permeabilities are required in the central portion of the reservoir.

Effective Permeability and Fluid Flow in Sandstone Containing Deformation Band Arrays: From Outcrop to Reservoir Scale

Kurt Sternlof, David Pollard, Mohammad Karimi-Fard, and Lou Durlofsky

School of Earth Sciences, Stanford University, Stanford, CA 94305

Extensive bleaching of the Jurassic eolian Navajo-Nugget-Aztec sandstone complex on and around the Colorado Plateau has been interpreted as evidence of hydrocarbon-related fluid flow on a massive scale during Late Cretaceous to Early Tertiary time. The close association of profound bleaching with structural and stratigraphic traps within these now exhumed sandstones suggests a combined paleo-reservoir potential far surpassing that of the Ghawar oil field in Saudi Arabia. Expansive outcrops of bleached Aztec Sandstone in the Valley of Fire, NV allow us to assess how one such paleo-reservoir would have performed if developed during K-T time.

Abundant geologic evidence indicates that pervasive arrays of relatively low porosity and low permeability deformation bands (DBs) comprised the dominant structural fabric then present in the otherwise high-porosity, medium-grained, sub-arkosic Aztec Sandstone. Using a combination of analytical methods and numerical techniques, we have calculated the net effect on sandstone permeability induced by systematic deformation band arrays at the outcrop scale. Our two-dimensional approach, based on homogenization theory, also provides a rigorous quantitative framework within which to extrapolate the effects of DB arrays to the reservoir-simulation scale. Our analysis of three characteristic DB patterns exposed in the Aztec—parallel, cross-hatch and anastomosing—indicates that they would reduce over all permeability by as much as two orders of magnitude, while inducing similar magnitudes of permeability anisotropy. These effects on permeability rival those routinely attributed to depositional heterogeneities (bedding, shale streak fraction, etc.).

In order to establish the spatial scale over which these permeability effects impact fluid flow, we are compiling detailed DB pattern maps of continuous outcrop areas covering tens of acres. Triangulated grids derived from these DB line maps, which reveal a dominant anastamosing pattern, provide the input for 2-D flow simulations based on a discrete fracture modeling approach that honors the effect of every band. Preliminary results reveal a profound influence on hydraulic communication between well pairs spaced hundreds of meters apart. For realistic values of average DB thickness and permeability, the pressure required to drive flow across the dominant band trend is about 3 times greater than would be expected in the absence of DBs, and about 50% more than needed to drive flow along the trend.

Importantly, the gross magnitude and character of the substantial reservoir-scale effects revealed by full flow simulation can be extrapolated from a representative DB pattern at the outcrop scale using our effective permeability assessment methods. We conclude that identifying DB arrays in the subsurface and accounting for their aggregate effects on fluid flow—even based on spatially limited data—would significantly improve simulation results and production management in many sandstone reservoirs.

Origin of Chemical Remanent Magnetizations:
Testing Diagenetic Remagnetization Mechanisms

R. D. Elmore[1], M. H. Engel[1] and A. Blumstein[1], W.C. Elliott[2], A. Basu[2]

[1]University of Oklahoma, Norman, OK, 73019
[2]Georgia State University, Atlanta, GA 30303

The objective of this study is to test models for the origin of widespread secondary magnetizations in the Mississippian Deseret Limestone and in marls on the Isle of Skye. The Delle Phosphatic Member of the Deseret Limestone is a source rock for hydrocarbons and modeling studies indicate it entered the oil window in the Early Cretaceous during the Sevier orogeny. Paleomagnetic and rock magnetic results from the Deseret Limestone and the stratigraphically equivalent Chainman Shale in central and western Utah indicate that the units contain two ancient magnetizations residing in magnetite. Burial temperatures are too low for the magnetizations to be thermoviscous in origin and they are interpreted to be chemical remanent magnetizations (CRMs). Fold tests from western Utah indicate the presence of a pre-folding Triassic to Jurassic CRM. Geochemical ($^{87}Sr/^{86}Sr$, $\delta^{13}C$, and $\delta^{18}O$) and petrographic analyses suggest that externally derived fluids did not alter these rocks. This CRM was acquired at the beginning of the oil window and is interpreted to be the result of burial diagenesis of organic matter. A second younger CRM in western/central Utah is apparently post-folding and is probably Late Cretaceous to Early Tertiary in age. Based on the thermal modeling, the timing overlaps with the oil window. These results are consistent with a connection between organic matter maturation and remagnetization. Modeling of the smectite-to-illite transformation in the Deseret Limestone suggests a mean age of illitization prior to acquisition of both CRMs although the range for illitization overlaps with the Triassic to Jurassic CRM.

The results of a previous study on Jurassic sedimentary rock of Skye, Scotland (Woods et al., 2002) supported a hypothesized connection between the smectite-to-illite conversion and magnetite authigenesis/remagnetization. The formation of diagenetic illite in marls may have been caused by heat and fluids associated with Tertiary (55 Ma) intrusions. A presence-absence test and the timing of acquisition of a dual polarity early Tertiary (50-60 Ma) CRM suggests that magnetite authigenesis is related to the smectite-to-illite conversion. To further test the connection between remagnetization and the smectite to illite conversion, K-Ar dating was used as an independent check on the paleomagnetic results. The measured K-Ar dates of illite and percentage of $2M_1$ illite both decrease with clay size fraction from 160-213 Ma (1-2 micron) to 101-105 Ma (< 0.25 micron). The age of diagenetic illite is derived by a non-linear extrapolation of measured K-Ar dates to 0% $2M_1$ illite (40- 67 Ma) and these extrapolated ages are concordant or slightly younger than the age of remagnetization and Tertiary intrusions. This analysis demonstrates the utility of a modified Illite Age Analysis technique to derive an age of diagenetic illite in marls and argillaceous limestones containing both detrital and diagenetic illite.

The results of this comparative study support the hypothesis that pervasive CRMs can be related to burial diagenetic processes in the Deseret Limestone. In addition, the results from Skye show that acquisition of both paleomagnetic and K-Ar ages can be used successfully to independently constrain the timing of such processes, which can aid in the interpretation of basin thermal histories and in hydrocarbon exploration efforts.

Geological, Geophysical, and Flow Modeling for a Mixed Tide- and Fluvial Influenced Delta, Wall Creek Member of the Frontier Formation, Wyoming, USA

Janok Bhattacharya[1], George McMechan[1], and Christopher White[2]

[1]*Department of Geology and Geophysics, U of Texas at Dallas, Richardson, TX*
[2]*Department of Petroleum Engineering, Louisiana State U, Baton Rouge, LA 70803*

Deltaic reservoirs comprise a major proportion of oil and gas reservoirs, aquifers, gas storage, and waste sequestration candidates in the United States and worldwide. These reservoirs commonly exhibit stratigraphic, lithologic, and petrophysical complexity that may affect flow behavior significantly: in the United States, 15 billion barrels of mobile oil remain unrecovered in fluvial-deltaic reservoirs.

An integrated geoscience study focuses on the Wall Creek Member of the Frontier Formation in central Wyoming. The goals are to improve models of delta architecture at a range of scales, formulate quantitative models for rock property distributions, assess the effects of observed features on flow behavior, and formulate methods and guidelines for use of these results in large-scale simulation models.

A regional stratigraphic study reveals the large-scale (tens of km) facies associations and variability within this top-truncated delta. Detailed studies (km-scale) at several localities use high-resolution digital photomosaics, measured sections, global positioning data, and digital surveying to create accurate geospatial models of bedding geometry and facies distribution. Finally, at the Raptor Ridge (circa 1-100 m) locality the aforementioned data are combined with ground-penetrating radar surveys, core samples, core analysis, field permeametry, and petrologic analyses. High-resolution (circa 10 μm) CT-scans are planned to compare pore structures of pervasively cemented rock types with "host" rock.

Two- and three-dimensional ground penetrating radar surveys are calibrated using core data and interpreted drawing on stratigraphy of adjacent near-strike and near-dip outcrop exposures. The results include a deterministic 3D stratigraphic framework; the area of principal interest is an 80 (dip) × 30 (strike) × ~12 (thick) m data volume (approximately 77×10^6 data locations). In addition, cluster analysis of core and radar data guides classification of lithofacies; the radar data are used to estimate the probability of a radar response at a given trace location assuming each of the discrete rock types.

The radar data are combined with facies proportion trends and autocovariances computed from the nearby outcrop exposures. The geostatistical model first uses the proportion trends as a geological prior to estimate update facies occurrence probabilities using truncated Gaussian simulation. In turn, these results are updated using cluster-derived facies classifications with Bayes' rule. The final results are optimal (kriging-like) or variance-preserving estimates of rock type occurrence; the estimates integrate the geologic prior, geospatial data from the outcrop and wells, and radar attributes.

The flow behavior of these models is examined using a suite of flow models selected by experimental design. This suite tests the importance of different data types – e.g., the impact of proportion curves vis-à-vis radar attributes. Finally, the best geostatistical models, as identified in the previous assessment, are used to derive response models for upscaled properties at a resolution suitable for field flow modeling. The responses include effective permeability, displacement endpoints, and shock velocities; the models depend on facies proportions, concretion occurrence, intrinsic rock properties, and engineering parameters including mean flow velocity.

Erosion Driven By Subsurface Flow: Theory and Experiment

Daniel H. Rothman[1], Alexander E. Lobkovsky[1], Arshad Kudrolli[2] and Braunen Smith[2]

[1]*Department of Earth, Atmospheric, and Planetary Sciences, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*
[2]*Department of Physics, Clark University, Worcester, Massachusetts 01610*

Erosion is generally thought to be driven by either overland flow or subsurface flow. The former case occurs when the shear stress imposed by a sheet flow exceeds a threshold. Erosion in the latter case - known as seepage erosion, or sapping - occurs when a subsurface flow emerges on the surface. In this case the eroding stresses derive not only from the resulting sheet flow but also the process of seepage itself. Here we summarize our studies of seepage erosion. We have constructed a laboratory analog of the process that exhibits many of the same features found in natural settings. Our objective is to understand as fully as possible the phenomena exhibited by our experiments.

Our experimental "sandpile" is composed of identical cohesionless glass beads. The sandpile is shaped into a wedge with slope s approximately one meter in length and width. Water enters the sandpile from below and seeps through it. A constant head at the inlet is maintained by keeping a constant water level H in a reservoir behind the wedge. The slope s and the water level H are the control parameters. A laser-aided tomographic imaging apparatus allows us to construct time-dependent two-dimensional elevation maps of the evolving surface.

For sufficiently small slopes and small water levels, the sandpile is immobile. Steeper slopes or greater water levels result in erosion of the pile in either of three ways: channelization, slumping, or fluidization. We have mapped out these regimes in the s-H parameter space, both experimentally and theoretically.

Our greatest interest is in the physical mechanisms that drive channelization. We currently focus on the dynamics of the amphitheater-shaped channel head. Our time-dependent measurements of the topography reveal that that the erosion rate depends quadratically on the gradient. Using this information we construct an equation for the erosion rate. This equation has the form of a driven Burgers equation. The coefficients of the equation carry information about the time averaged microscopic physics of the small granular avalanches driven by the water flux. Augmented by appropriate boundary conditions and driving forces, our erosion equation predicts the shape of the cross-sectional channel topography as well as its time-dependent growth. Preliminary comparisons of the predicted channel geometry with real, field-scale, seepage channels indicate that our theoretical model may help reveal quantitative aspects of the subsurface flows that erode the channels.

Pore Scale Imaging and Fluid Flow in Geomaterials

J. T. Fredrich[1] and Teng-fong Wong[2]

[1]*Sandia National Laboratories, Albuquerque, NM 87185*
[2]*SUNY at Stony Brook, Stony Brook, NY 11794*

Geologic materials exhibit geometrically complex microstructures that control physical and mechanical properties at the macroscale. The past decade has seen development of new experimental techniques that enable direct high-resolution three-dimensional imaging of the microscopic structure of geomaterials. We discuss the advantages and disadvantages that the two highest fidelity methods, synchrotron computed microtomography and laser scanning confocal microscopy, present in the specific context of microscale imaging, contrast these modern techniques with conventional serial sectioning techniques, and describe unique experiments possible with the current generation of laser scanning confocal microscopes. The availability of high-quality three-dimensional image data, coupled with advances in numerical simulation methods, offers unprecedented opportunities for the prediction of bulk physical and mechanical properties directly from microscale image data. Using three-dimensional image data obtained for several natural and synthetic sandstones, we explore fundamental issues related to representative volumes and length scales necessary to characterize geometrically complex porous media and enable accurate prediction of physical properties at the macroscale. We consider several data sets collected during synchrotron computed microtomography experiments performed at the GSECARS 13-BM beamline at the Advanced Photon Source. Four data sets were collected for a series of synthetic sandstones sintered to differing bulk densities, with each of the data sets containing ~30 million voxels (approximately 250×250×500), with voxel resolution of 3.34 micron. The other four data sets were collected from a single sample of a natural sandstone, Castlegate. Three data sets were collected from different sub-volumes within this sample, with each data set containing ~90 million voxels (approximately 424×424×500), with voxel resolution of 3.34 micron. A fourth data set was collected for the exact same volume as one of the three previously imaged sub-volumes, but at twice the resolution. This data set contains just over a half billion voxels (800×800×800), with voxel resolution of 1.67 micron. Following meticulous processing to extract binary descriptions of the two-phase structure, the data are analyzed to extract porosity and specific surface area, and applied directly in numerical simulations of single phase fluid flow performed using the lattice Boltzmann method. Our specific implementation of the LB method enables massively parallel simulations of volumetric data sets greater than 1000^3 (10^9) voxels. The numerical simulations are used to calculate macroscopic permeability, which can be compared to experimental measurements of intrinsic permeability performed at bench conditions (a few hundred psi) on core samples (1 × 2 inch). The results offer insight into the significance of the micron-scale roughness of the pore-grain interface, and the locally heterogeneous nature of pore-scale flow in geomaterials.

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3D Microtomographic Analysis of Fluid Displacement in Berea Cores

W.B. Lindquist,[1] M. Prodanovic,[1] and R.S. Seright[2]

[1]*Department of Applied Mathematics and Statistics, Stony Brook University, Stony Brook, NY 11794*
[2] *New Mexico Petroleum Recovery Research Center, New Mexico Institute of Mining and Technology, 801 Leroy Place, Socorro, NM 87801*

We report on three-dimensional pore-scale medium characterization and fluid partitioning in a Berea (water wet) core. X-ray computed microtomography employing X-ray attenuating dopants is used to obtain three-dimensional images of two-phase distributions at residual fluid conditions in the pore space (Fig. 1). Employing numerical image processing algorithms based upon computational geometry to identify individual pores, throats, and fluid "blobs", we extract water and oil distributions at the level of individual pores in imbibition and drainage displacements.

We present results on the characterization of the pore space in Berea sandstone, including distributions for pore volume, pore surface area, throat area, and principal direction diameters for pores and throats. Our findings indicate that both pore volume and pore surface area are log-normally distributed in Berea sandstone with respective mean values of 0.00026 mm^3 and 0.043 mm^2. The distribution of throat areas is much broader, with mean value of 0.0006 mm^2.

Our fluid distribution studies target the effects on residual fluid distribution due to the injection and gelation of a water-based gel. We present results on distribution of the oil and water phases at residual conditions both before and after emplacement of the water-based gel. In extensive studies of Berea cores it has been observed that introducing water-based gels in the displacement process (for example, in water shut-off treatment of production wells) reduces permeability to water more than to oil. A number of micro-scale mechanisms have been proposed for this disproportionate permeability reduction. Our results provide supporting evidence for the involvement of gel dehydration and oil trapping while discounting gel blockage in throats as contributing mechanisms. Our images also reveal mobilization of residual oil upon injection of the aqueous based gel phase. Such mobilization has been observed previously and is believed to result from the non-Newtonian properties of the gel phase (rather than, for example, from the high viscosity of the gel).

Reconstruction of individual throats in the rock enables simulation of flow through individual throat structures. We report on the variation of absolute permeabilities computed by lattice Boltzmann methods for an ensemble of 700 throats reconstructed from the sandstone core image.

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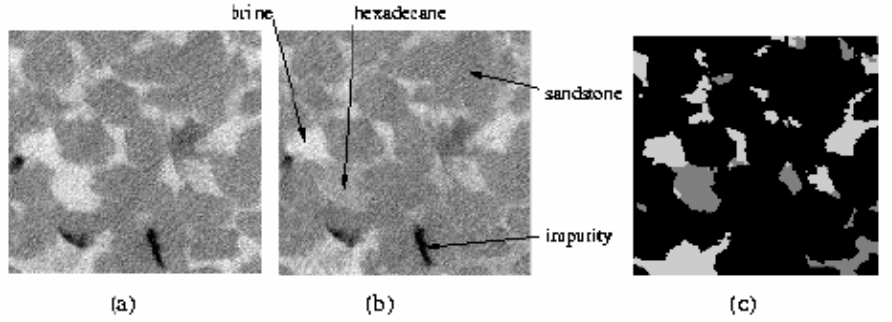

FIG. 1. A sub-region of the core image at a) water saturated and b) residual oil conditions. c) Phase identification results for b).

Lattice Boltzmann Simulation of NMR Phenomena in Porous Media

Mounira Boudjema and Katherine McCall

University of Nevada, Reno, NV 89557

In a Nuclear Magnetic Resonance (NMR) experiment the magnetization of a system is set away from thermal equilibrium at t=0 and monitored over time as it returns to thermal equilibrium. In a porous medium the magnetization resides in the pore fluid. In returning to thermal equilibrium it encounters the pore walls, senses the flow of the pore fluid, etc. Thus the data, magnetization as a function of time, carries information about the nature of the pore space/fluid flow at the "microscopic" level. This information is extracted from the magnetization with a suitable model. The complexity of realistic models of porous media precludes establishing their efficacy analytically. Lattice Boltzmann methods offer a facile computational scheme for the simulation of the behavior of magnetization in the presence of elaborate NMR experimental manipulations and realistic pore spaces.

Pore-scale Simulation Tools for Understanding and Predicting Physical Properties of Rocks

Amos Nur and Youngseuk Keehm

Stanford Rock Physics Lab, Stanford University, Stanford, CA 94305

The earth sciences are undergoing a gradual but massive shift from *description* of the earth and earth systems, toward *process modeling and simulation*. This shift is very challenging because the underlying physical and chemical processes are often nonlinear and coupled. In addition, we are especially challenged when the processes take place in strongly heterogeneous systems. One example is multiphase fluid flow in rocks, which is a nonlinear, coupled and time-dependent problem and occurs in complex porous systems. To understand and simulate these complex processes, the knowledge of underlying pore-scale processes is essential. To this end, we have initiated computational rock physics to rigorously simulate rock/reservoir properties. The computational rock physics framework is based on digital representations of rocks, which consist of minerals and fluids, and may evolve with time. It also contains modular physical property simulators, with which we directly simulate physical properties of rocks. This computational environment significantly complements the physical laboratory: (1) rigorous prediction of the physical properties, (2) interrelations among the different rock properties using shared digital porous media, and (3) simulation of dynamic problems with multiple physical responses. The primary objective of the framework is building rigorous pore-scale simulators for predicting physical properties of rocks with realistic pore microstructures. We pay special attentions to three aspects in developing the rigorous pore-scale simulators: reliability, efficiency and ability to handle complex micro-geometry.

We have shown results for single-phase and two-phase flow simulations using the Lattice-Boltzmann method in the last meeting. To overcome the long calculation time of flow simulation, we have now implemented efficient parallel flow simulators by creating four optimization techniques customized for the Lattice-Boltzmann algorithm. The optimized two-phase code runs 12 times faster with 14 processors than its serial counterpart, while the generic parallel code is only 4 times faster. With the parallel simulators, we can perform flow simulations on more realistic, complex and bigger pore geometry. Pore-scale simulators for elastic and electrical properties using the finite-element method were also added to the computational rock physics framework. We made extra efforts for the new simulators to handle the same microgeometry used for fluid flow simulations without modification or simplification. The new computational modules were tested against the lab data, and showed very good agreement. These pore-scale simulators give us a better link to reservoir management. We investigated interrelations of physical properties under different diagenesis histories. We found that the relations between electrical conductivity and permeability show very distinct trends in different diagenetic models. Partial saturation was also modeled using the pore-scale simulators, and we will present the results with permeability and electrical conductivity. Diagenesis and partial-saturation modeling showed that the pore-scale simulation environment provides rigorous links to understanding and modeling geological processes.

Theory for Quartz Cementation in Structurally Deformed Sandstones

R. H. Lander[1], L. M. Bonnell[1], S. E. Laubach[2], J. E. Olson[3]

[1]Geocosm LLC, [2]Bureau of Economic Geology, [3]Petroleum & Geosystems Engineering, The University of Texas at Austin

A comprehensive theory for quartz cementation must account for variations in the abundance and morphologies of cement in undeformed sandstones as well as in fractures of all scales. Our approach toward developing such a theory is to extend existing kinetic models by rigorously simulating the crystal growth anisotropy and nucleation surface area.

For our analysis we assume that the rate limiting control on quartz cementation is the crystal precipitation rate (Walderhaug 1994, 1996, 2000). In a strict sense this assumption does not address whether the silica is derived from local diffusion or larger scale fluid advection but instead simply considers that dissolved silica is supplied at a rate that equals or exceeds the rate at which the crystals can precipitate. This assumption is reasonable for quartz cementation in near neutral pH fluids at temperatures in excess of ~80 °C but is not applicable to quartz precipitation in highly supersaturated fluids (e.g., in silcretes, saline-alkaline lakes, or in the presence of biogenic opal).

We assessed the predictive accuracy of a kinetic model for quartz cement abundance in undeformed sandstones. The model (Touchstone™ version 5.0) considers the temperature effect on precipitation rates, the increase in surface area normalized rates of precipitation with nucleation surface area that have been documented in natural and synthetic quartz overgrowths (Makowitz and Sibley 2001, Bonnell and Lander in preparation, Lander et al in preparation), and the nucleation surface area and how it varies with sandstone texture, depositional composition, and diagenetic alteration. Quartz cement abundances are predicted to within four bulk volume percent of the measured values for more than 90% of structurally undeformed sandstone samples from diverse basin settings (rift, wrench, foreland/thrust belt, and cratonic), compositions (quartzarenite to litharenite to subarkose), thermal histories (maximum temperatures ranging from 108 to 244 °C for samples with Ordovician to Miocene depositional ages), and fluid overpressures (from hydrostatic pressure to near fracture gradient fluid overpressures) (Bonnell and Lander in preparation).

We have extended this quartz modeling approach to explicitly account for the following effects of particular importance in structurally deformed sandstones: (1) substantially greater growth rates on surfaces that grow parallel to the c-crystallographic axis (pyramidal faces) compared to along the a-crystallographic axes (prismatic faces), (2) the order of magnitude increase in precipitation rate on non-euhedral surfaces compared to euhedral surfaces growing along the same crystallographic orientations (Lander et al in preparation), and (3) the complex interaction of repeated fracturing and cementation on nucleation surface area.

Preliminary results obtained using a 2D model incorporating these effects (Prism™) reproduces quartz morphologies in fractures of varying scales as well as in pores within undeformed sandstones. Results indicate that the abundance and morphology of quartz cement within fractures depend on the relative rates of quartz precipitation and fracture opening, the geometries and sizes of grain surfaces and pores, and the orientations of crystallographic axes with respect to fractures. Pervasive quartz sealing of fractures occurs in the simulations when the rate of crystal growth on surfaces of the slowest growing type (along the a-crystallographic axis) exceeds the net rate of fracture opening. Euhedral quartz crystals rim otherwise open fractures when the rate of fracture opening exceeds the fastest rate of quartz crystal

growth (on non-euhedral surfaces that grow parallel to the c-crystallographic axis). Simulations suggest that quartz bridges form where the following conditions are met:

- The c-crystallographic axis is near perpendicular to the fracture plane for monocrystalline grains bisected by the fracture.
- Increases in fracture apertures are small for individual fracture events (e.g., microns to tens of microns),
- Integrated over geologic time scales, the rate of kinematic aperture increase is less than the rate of precipitation along the quartz c-axis on non-euhedral surfaces (the fastest growth rate) but greater than a-axis precipitation rates, and
- Fracturing of bridged quartz crystals periodically creates new non-euhedral nucleation surfaces.

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Evolution of Fracture Permeability

Stephen Brown[1] and Harlan Stockman[2]

[1]*New England Research, White River Junction, VT 05001*
[2] *Geochemistry Department, Sandia National Laboratory, Albuquerque, NM 87185*

Pore fluid flow within fractured rocks is a subject of primary importance to various fields of study including hazardous waste isolation and remediation, oil and gas production, geothermal energy extraction, and formation of vein fillings and ore deposits. For these reasons, considerable effort has been directed toward the characterization and modeling of flow in fractures and fracture systems. We are investigating the complex active chemical interaction between pore fluid and fractures that causes the fluid composition and fracture surface topography of these systems to change over time.

Our experimental model consists of $CaSO_4$ samples pressed with a constant force against an inert textured fracture surface. Pore fluids ranging from unsaturated to supersaturated, which are at a variety of flow rates, are introduced to one end of the sample in order to actively alter the topography of the $CaSO_4$ surface. Using a laser profiler, we are able to quantitatively monitor the changing surface topography over time as it relates to the measured sample permeability and calcium saturation of the pore fluid. These methods allow us to create and analyze many features seen in natural fractures, including high-flow dissolution channels, plateaus, and caverns formed from precipitate. In addition, the laser profile of the sample surface can be used to produce a map of aperture across the sample. Using this information, we have applied numerical modeling via finite difference and lattice Boltzmann (LB) methods to calculate pore fluid flow direction and magnitude over the entire sample surface.

We find that when experimental parameters (e.g. initial surface topography, flow rate history, and total experiment time) are duplicated, the topography developed on the plaster sample is reproducible. The flow channel networks, as observed visually and through numerical simulations, evolves from a homogeneous system to one more (self) organized and complex. The permeability initially drops as the experiment begins and the surfaces settle into place, then gradually rises with several further smaller decreases as some supporting asperities are destroyed. LB methods predict the formation of major dissolution features, such as long "stringers" in the lee of obstacles.

LB predicts that dendrites may grow along fracture surfaces under saturated conditions. This form of growth can be the major cause of decreasing permeability, even when the added solid fraction is small. LB predicts dendrites will grow toward time-varying regions of fast flow, a prediction borne out by previously published experiments.

Dissolution of Single Fractures:
The Role of Aperture Variability and Reactive Fluid Flow on Permeability Evolution

Russell L. Detwiler[1], Souheil Ezzedine[1], and Harihar Rajaram[2]

[1]Lawrence Livermore National Laboratory, Livermore, CA 94551
[2]University of Colorado, Boulder, CO 80309

Fractures typically comprise only a small portion of reservoir porosity yet can provide dominant pathways for flow and transport. Because of the strong dependence of fracture permeability on local fracture apertures, chemical alteration (precipitation/dissolution) of fracture surfaces may strongly influence the flow and transport properties of individual fractures. The spatial variability of fracture apertures, which leads to channeled flow and non-uniform surface reactions, complicates efforts to predict the role of chemical alteration on fracture permeability. Using an integrated experimental and computational approach we have investigated the combined influence of aperture variability and reactive fluid flow on the evolution of permeability in single fractures.

We have developed a novel approach for conducting systematic and quantitative dissolution experiments in variable-aperture analog fractures. Fractures created by mating an inert textured surface (glass) with a reactive smooth surface (potassium dihydrogen phosphate) allow us to reproduce initial fracture geometries in multiple experiments. Furthermore, because both fracture surfaces are transparent, we can use well-established light-transmission techniques to accurately measure changes in fracture aperture over the entire flow field (10 x 15 cm) at high spatial resolutions (83 x 83 μm pixels) throughout the duration of each experiment. Experiments at different flow rates exhibit quite different dissolution patterns in the reactive surface: at slow flow rate (Peclet number (Pe) = $V\langle b\rangle/D_m = 54$, where V is the mean flow velocity, $\langle b\rangle$ is the mean aperture and D_m is the molecular diffusion coefficient of the dissolved mineral) distinct dissolution channels form until one dominant channel breaks through to the outflow end of the fracture, whereas at higher flow rate (Pe=216), dissolution occurs more uniformly across the fracture, with small aperture regions dissolving most quickly. The effect of these contrasting dissolution patterns is that equal changes in mean fracture aperture result in significantly different changes in fracture permeability.

Using the quantitative experimental results, we have evaluated and refined a computational model that solves two-dimensional approximations of the flow and reactive transport equations to efficiently simulate dissolution over the entire fracture domain (1160 x 1800 grid blocks). The model predicts the differences in the dissolution patterns within the fracture and predicts the relative changes in permeability, but underestimates the magnitude of the permeability changes. We use this model to explore the influence of Pe over a broader range of values through a series of parametric simulations in a series of synthetic correlated random aperture fields.

Coupled Chemical-mechanical Effects and their Influence on the Transport Properties of Fractures in Rock

Derek Elsworth, Amir Polak, Hideaki Yasuhara, and Abraham Grader

Penn State University, University Park, PA 16802

Anomalous changes in permeability are observed in fractures circulated by fluids undersaturated with respect to the mineral host. Under net dissolution and net removal of mineral mass, fractures may alternately gape or seal, depending on the prevailing mechanical and chemical conditions. The influence on transport properties is observed to be large, rapid, and irreversible: permeabilities may change by two orders of magnitude in a month, and the direction of permeability change may switch spontaneously, for no apparent change in environmental forcing. These behaviours are apparent in continuous circulation experiments conducted on fractures in novaculite and limestone, intermittently imaged by X-ray CT. In novaculite [Figure 1] permeability *reduces* by two orders of magnitude as silica is *net removed* from the sample. Surprisingly, these changes can occur at modest temperatures (~80°C) and stresses (~3.5 MPa), for water circulation at constant flow rate (2 cc/min), where compaction progresses as temperatures are incremented. Isothermal (~20°C) circulation tests in limestone show similar compaction driven by pressure solution [Figure 2]. Where circulation remains undersaturated in Ca, the change in permeability spontaneously switches from net reduction to net increase as a wormhole forms. The surprising magnitude and rapidity of these changes are explained in the context of the competition between stress- and chemistry-mediated effects.

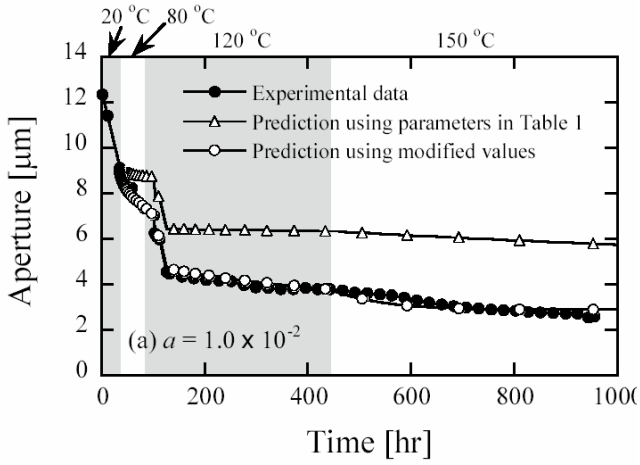

Figure 1. Change in aperture for circulation of water at 2 cc/min in novaculite at incremented temperatures. Experimental data filled circles. Model results as open triangles and circles.

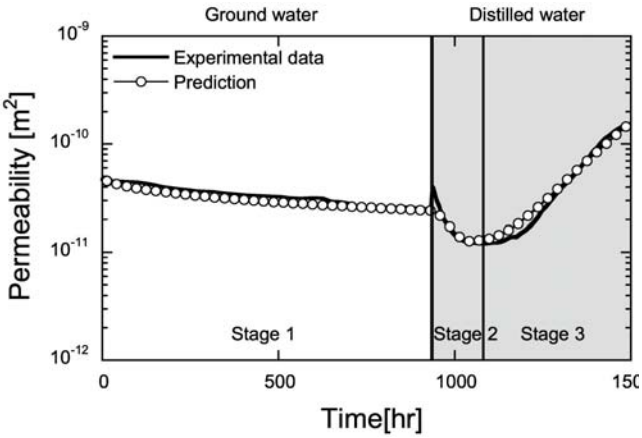

Figure 2. Change in permeability with time for continuous flow at 2 cc/min through a fracture in limestone. Test at invariant low temperatures (~20°C) and effective stresses (~3.5 MPa). Influent water changed at 935 h from groundwater (pH~8, unshaded panel) to distilled water (pH~6, shaded). At 935 h a brief sharp increase in permeability, is followed by a coherent decrease in permeability, that ultimately arrests as a single flow conduit develops, and permeability climbs.

Microscopic Simulations of Dissolution in Fractured Rocks

Anthony JC Ladd

Department of Chemical Engineering, University of Florida, Gainesville, FL 32611

Microscopic simulations of fracture dissolution are reported, taking account of the explicit topography of the pore space, the transport of reactants and products, and the chemical kinetics at the solid surfaces. A three dimensional numerical model has been constructed, in which the fluid velocity field is calculated with an implicit lattice-Boltzmann method, and the transport of dissolved species is modeled by an innovative random walk algorithm that incorporates the chemical kinetics at the solid surfaces. The model contains no free parameters or semi-empirical mass-transfer coefficients. The simulated morphological changes in a complex fracture are compared with recent laboratory experiments with the same initial topography.

Transport Properties of Rough, Self-Affine Fractures

German Drazer and Joel Koplik

Levich Institute, City College of CUNY, New York, NY 10031

We present numerical results on the transport properties of single rock fractures. Geological fractures present rough surfaces with long-range spatial correlations in the height distribution, and experiments show that fracture surfaces can be described as self-affine fractals. The self-affine topography of rock fractures implies that they do not have a characteristic length and that parameters such as surface roughness depend on the length scale of the problem. In our work, we consider fluid flow in fractures *joints*, which present a strong correlation between the opposite surfaces of the fracture, and which can therefore be modeled as the gap between a self-affine surface and its exact replica, translated in the normal direction. In addition, we also investigate the effects of possible shear-displacements between opposite surfaces of the fracture, which may occur during the fracturing process, by introducing a lateral shift on the top surface.

First, we investigate the permeability to fluid flow, and its dependence on the aperture, in *narrow* fractures, for which the surface variations in height are large compared to the gap between surfaces. In this case, although the lubrication approximation fails to describe the effects of surface roughness, we show that a simple correction accounting for the effective *tortuosity* of the system is able to capture the correct scaling of the permeability on the aperture. We then show that a shear-displacement, between the surfaces of the fracture, induces a remarkable anisotropy in the permeability of the fractures, which has also been observed in recent experiments in laboratory model fractures. Surprisingly, while the permeability is significantly reduced in the direction of the shear displacement, there is little effect in the orthogonal direction, where the permeability even increases slightly. Finally, we show that the permeability of fully three-dimensional fractures can be bounded by the permeability in two-dimensional fracture profiles.

We also investigate the dispersion of tracer particles advected through the fractures. We first show that, again, a simple tortuosity factor is able to capture the reduction in self-diffusivity as the fracture gap decreases. Then, in the presence of convection, Taylor-dispersion becomes dominant, and we shall describe the effects of surface roughness, that creating low velocity regions and tortuous path for fluid flow. Finally, we investigate the evolution of a displacement front in such a fracture, and show how it directly reflects the complex geometry of the fracture, displaying the permeability anisotropy at large length scales, while inheriting the self-affine character of the fracture walls in an intermediate scaling range.

Fundamental Studies of Two-phase Flow, Transport and Inter-phase Mass Transfer in Rock Fractures

Harihar Rajaram[1], Robert J. Glass[2], Russell Detwiler[3], Michael J. Nicholl[4], Matthew Bliss[1]

[1]*University of Colorado, Boulder, CO*
[2]*Sandia National Laboratory, Albuquerque, NM*
[3]*Lawrence Livermore National Laboratory, Livermore, CA*
[4]*University of Nevada, Las Vegas, NV*

The objective of this project is to develop a quantitative understanding of the critical processes controlling two-phase flow and transport in rock fractures. Fundamental results may be abstracted for applications in petroleum engineering, radioactive waste isolation and CO_2 sequestration. Our previous research identified the importance of phase structure in controlling system behavior. We have developed unique experimental systems to create and measure a wide range of phase structures. Flow and transport experiments through these structures facilitated concurrent model development. Current efforts focus on developing parametric relationships for flow, transport and inter-phase mass transfer associated with the satiated state, where the invading phase completely entraps the defending phase. In experiments, this state is attained relatively quickly when capillary forces dominate, and persists for long durations in the absence of inter-phase mass transfer. It is thus important in a variety of practical contexts.

The areal saturation (S_f) of the flowing phase at satiation is shown to depend on the ratio of two dimensionless parameters (C/δ, where the curvature number C, weighs the mean in-plane interfacial curvature relative to the mean out-of-plane interfacial curvature, and δ, the coefficient of variation of the aperture field, represents the strength of interface roughening induced by aperture variations). The ratio C/δ represents the competition between the smoothing influence of in-plane curvature and the roughening influence of random aperture variability. As C/δ goes to zero, behavior is as in standard invasion percolation (no influence of in-plane curvature) within a correlated field, and S_f has a rather low value of about 0.37. As C/δ increases above ~ 0.1, S_f increases, approaching 1 (i.e. no entrapment) for very large C/δ ~10. These results were published in Physical Review E 68, 061110 (2003).

A parametric relationship for the satiated relative permeability has been developed based on detailed computational studies. The computational results were interpreted using concepts from effective medium and continuum percolation theory, leading to a physically appealing expression, incorporating the influence of both S_f and δ. Results have been submitted to Physical Review E. Experimental and computational studies of solute transport have revealed that within realistic ranges of Peclet number (Pe) in two-phase systems, the dominant dispersive mechanism can be molecular diffusion, geometric dispersion or Taylor dispersion. Efforts are underway to develop a fracture-scale effective transport equation with effective parameters dependent on S_f, δ and Pe.

Detailed experimental and computational studies have led to the development of an accurate and robust model for the dissolution of an entrapped phase within a variable-aperture fracture. This model couples flow, transport and alteration of entrapped phase geometry through a quasi-steady state approximation. Parametric studies based on this computational model have led to a comprehensive understanding of dissolution beginning from a satiated state. The overall dissolution process is controlled largely by the areal saturation S_f

Infiltration Flow Path Distributions in Unsaturated Rocks

Tetsu K. Tokunaga

Earth Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720

Spatial distributions of infiltration flow paths through rock formations are complex networks that determine flow velocities, control rates of natural geochemical reactions in the subsurface, as well as rates of contaminant transport to underlying ground water. Despite these important consequences, distributions of infiltration paths and locally fast seepage rates through rocks are not well understood. Although a number of approaches to predicting infiltration through rock formations involve modifications of analyses applicable to soils, it has also long been recognized that unsaturated rocks are hydraulically very different from fine-grained porous media. With this in mind, our recent BES research has progressed through 3 stages; (1) delineate upper scale limits for capillary influences on unsaturated hydraulic phenomena, (2) conduct laboratory experiments to determine flow path distributions through unsaturated rocks, and (3) develop experimentally tested models for predicting distributions of infiltration flow paths and rates in rocks.

Upper scale limit for capillarity in unsaturated media:

Hysteresis in the relation between water saturation and matric potential is regarded as a basic aspect of unsaturated porous media. However, the nature of an upper length scale limit for saturation hysteresis has not been previously quantified. Because hysteresis depends on whether or not capillary rise occurs at the grain-scale, this criterion was used to predict influences of grain-size, surface tension, fluid densities, and acceleration. The Haines number (Ha), comprised of the aforementioned variables, is proposed as a dimensionless number useful for separating hysteretic ($Ha < 15$) versus nonhysteretic ($Ha > 15$) behavior. Vanishing of hysteresis was predicted to occur for grain-sizes greater than 10.4 ± 0.5 mm, for water-air systems under the acceleration of ordinary gravity, based on Miller-Miller scaling and Haines' original model for hysteresis. Disappearance of hysteresis was tested through measurements on sands and gravels, with and without surfactants. The experiments completed in this study support our predictions and show that hysteresis is not a fundamental feature of unsaturated porous media.

Flow path distributions in unsaturated rock deposits:

Water infiltration experiments in unsaturated rock deposits permit quantification of flow path distributions, have advantages over laboratory and field experiments in fractured rocks, and providing new insights relevant to predicting flow and transport. Experiments have been conducted on 4 different rock types and system scales ranging from 1 to 30 rock layers. Our experiments showed that infiltration through rocks conforms to no previously reported behavior in soils, and that flow paths do not progressively converge into fewer and fewer flow paths. Instead, a fundamentally different hydraulic structure develops, having an exponential flux distribution, with the characteristic scale determined by the characteristic rock block size.

Statistical mechanical flow path model:

Although the phenomena are very different, the evolution of flow path distributions and local seepage rate distributions is predictable based on a model for quantized energy distributions in solids. All of the above studies are aimed at linking microscale hydraulics to a field-scale understanding of reactive transport in unsaturated rock formations, including predicting rates of contaminant transport to groundwaters.

Colloid Fate and Transport in Unsaturated Porous Media

Jiamin Wan

Earth Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720

Colloids are particles ranging in size from 1 nm to a few μm, including fine minerals, organic macromolecules, and microorganisms. Although it has been widely reported that transport of low-solubility contaminants in subsurface environments can be enhanced through association with mobile colloids, quantification of such effects remain challenging. This is especially true in the unsaturated zone through which contaminants must traverse before reaching groundwater. During the previous and the current funding cycles, we have made significant progress on improving fundamental understanding in the area of colloid fate and transport in unsaturated porous media. We will present original results from three aspects of our ongoing research.

Film-straining model of colloid transport in unsaturated porous media:

Models for colloid transport in subsurface environments are based on earlier developments in colloid filtration theory, which is limited to a single fluid phase but not directly applicable to transport through the vadose zone. We introduced the concept of "film straining" as the main colloid transport mechanism in partially saturated media that differs from transport under saturated conditions. We also developed a predictive model by introducing the concepts of "critical saturation" and "colloid size to film thickness ratio". These concepts and model have been well adopted by the research community in this field. However, the model has been tested only macroscopically (through one-dimensional sand columns) and in ideal porous media (uniform grain sizes). We do not yet understand colloid film straining at pore and grain scales. The latest progress on colloid film straining obtained through a pore scale visualization will be presented.

Nanoparticles in subsurface environments: abundance and transport of the mobile fraction:

The current growing interests in nanomaterials and nanotechnology have provided the geoscience community with incentive to evaluate our understanding of nanoscale phenomena in many of the Earth's natural processes. Among the many gaps in understanding nanoscale processes, there are two fundamental questions that are broadly important to subsurface environments.. How abundant are nanoparticles in the subsurface? How far can they move? In order to obtain inventories of mobile nanoparticles for common subsurface environments, studies were conducted on sediments obtained from a variety of DOE's contaminated sites including the Hanford, Livermore, Oak Ridge, and Savannah River. Despite experimental difficulties in quantifying the mass of nanoparticles (< 100 nm), our results show that nanoparticles exist in all the sediments studied. The mass percentage of nanoparticle fraction is proportional to clay fraction (< 2 μm) of the sediments. The mobility of the nano-fraction is largely controlled by pH of the pore solution. Under hydrodynamic conditions representative of the subsurface, there was no measurable nanoparticle release and transport at pH values below 7.0. To our knowledge these are the first quantitative information on subsurface nanoparticle inventory and mobility.

Colloids at waste plume fronts:

We have recently revealed a striking phenomenon of colloid formation and transport during waste solution infiltration into sediments. Colloid formation and transport was thousands of times higher within a narrow zone at the moving plume front than in the plume body and the leaching stage. The newly formed plume front colloids were primarily in the size range from tens of nm to a few μm. This plume front colloid generation phenomenon can occur under a wide range of conditions, with the only necessary condition being that of high

ionic strength in the waste plume. The rapid and completed Na^{+} replacement of exchangeable Ca^{2+} and Mg^{2+} from the sediment caused accumulation of these divalent cations at the moving plume front. Precipitation of supersaturated Ca^{2+}/Mg^{2+}-bearing minerals caused dramatic pH reduction at the plume front. In turn, the reduced pH caused precipitation of other solid phases. Because of the large amounts of suspended colloids generated, this phenomenon could significantly affect the fate and transport of the contaminant trace elements contained within the waste plume.

Coupling of Dynamic Stress to Porous Fluid Flow and Colloid Behavior: Experimental Observations from Sub-Pore to Core Scales

Peter M. Roberts, Amr I. Abdel-Fattah and Joel Duran

Los Alamos National Laboratory, Los Alamos, NM 87545

Dynamic stress oscillations are known to induce observable changes in fluid-flow behavior in porous media. Different types and degrees of flow changes will occur with different combinations of dynamic-stress parameters, such as frequency, amplitude, wave mode and duration, and with the medium properties, such as permeability, elastic moduli, sub-pore-size particle (colloid) content, mineralogy, fluid saturation and ionic strength. Stress waves over a wide range of frequencies (roughly 1 Hz to 50 kHz) have been observed to influence porous fluid-flow behavior in the Earth and geomaterials over a similarly wide range of scale lengths (microns to kilometers). Published examples include oil reservoir production increases induced by seismic (1 to 500 Hz) waves and mobilizing colloidal clay particles in sandstone cores by ultrasonic (10 to 50 kHz) energy. Other potential applications include accelerated contaminant extraction from groundwater aquifers, and controlling colloid transport at waste facilities. The majority of field-scale observations to date have been mixed, unpredictable and anecdotal because the physical mechanisms coupling *stress-wave propagation* to *colloid electrokinetics* and *fluid-flow dynamics* in porous media are not understood. This project focuses on laboratory experimental research designed to improve our understanding of the coupling between these three scientific disciplines. One of several mechanisms being studied in detail is nonlinear coupling of dynamic stress energy to sub-pore-size colloid behavior. This is an important mechanism because the distribution of colloids in a porous medium will directly affect its permeability.

Colloid behavior in high-frequency acoustic fields is being characterized with a microscopic, video image-processing system, focused on a glass flow-visualization cell that contains known colloid/fluid suspensions. Using 0.5- to 3-micron diameter polystyrene spheres suspended in 0 to 0.1 *M* aqueous solution, three types of behavior were observed in the video images when the glass cell was excited with acoustic energy at 100 kHz to 10 MHz: 1) Colloid conglomeration and alignment at specific locations in the cell, 2) Induced fluid convection and colloid entrainment, and 3) Changes in colloid attachment to and detachment from the glass cell surfaces. Initial image-processing-based analysis of acoustically-induced colloid/surface detachment events indicated that acoustics not only increases particle detachment, but may also permanently "deactivate" colloid attachment (or "active") sites on the glass cell surface. It was also observed that the three types of colloid behavior are sensitive to a large number of parameters, including colloid size, ionic strength of the fluid, and acoustic frequency.

Effects of dynamic stress on core-scale (cm to m) bulk-fluid porous flow are being investigated in the seismic range of frequencies (1-500 Hz), using a core-holder apparatus that mechanically strains 2.54-cm-diameter porous rock samples during constant-rate fluid flow. During single-phase brine flow through Berea sandstone, axial stress oscillations at 50 Hz increased the absolute permeability of the rock by 10 to 20 percent. This was caused by mobilizing in-situ clay colloids that were partially plugging the pore throats. During 2-phase, steady-state, constant-rate flow of oil-plus-brine and decane-plus-brine mixtures, dynamic stress at 25 to 75 Hz caused significant changes in the bulk fluid pressure drop across the core. This may indicate that relative changes in the mobility of wetting versus non-wetting fluid phases were induced by the dynamic stress. Under the specific experimental conditions used, sub-pore-scale colloid

perturbation and altered wettability are possible physical mechanisms that can explain the core-scale results.

Participants:

Amr I. Addel-Fattah, Los Alamos National Laboratory

Martin Appold, University of Missouri

Atilla Aydin, Stanford University

Roger Beckie, University of British Columbia

Edward Bolton, Yale University

Mounira Boudjema, University of Nevada, Reno

Stephen Brown, New England Research

Gilles Bussod, New England Research

Akhil Datta-Gupta, Texas A&M University

Russell Detwiler, Lawrence Livermore National Laboratory

German Drazer, City College of New York

Crawford Elliot, Georgia State University

Douglas Elmore, University of Oklahoma

Derek Elsworth, Penn State University

Ronald Falta, Clemson University

Joanne Fredrich, Sandia National Laboratory

Grant Garven, Johns Hopkins University

Marios Ioannidis, University of Waterloo

Youngseuk Keehm, Stanford University

Mack Kennedy, Lawrence Berkeley National Laboratory

Michael J. King, BP

Joel Koplik, City College of New York

Arshad Kudroli, Clark University

Tony Ladd, University of Florida

Rob Lander, Geocosm L.L.C.

Stephen Laubach, University of Texas, Bureau of Economic Geology

David Lesmes, Department of Energy

Brent Lindquist, State University of New York and Stony Brook

Diane Marceau, Department of Energy

Katherine McCall, University of Nevada, Reno

John Miller, Department of Energy

Amos Nur, Stanford University

David Pollard, Stanford University

Jonathan Price, Rensselaer Polytechnic Institute

Karsten Pruess, Lawrence Berkeley National Laboratory

Harihar Rajaram, University of Colorado

Chris Reddy, Woods Hole Oceanographic Institution

Peter Roberts, Los Alamos National Laboratory

Daniel Rothman, Massachusetts Institute of Technology

Robert A. Sanford, University of Illinois at Urbana-Champaign

Kurt Sternlof, Stanford University

Harlan Stockman, Sandia National Laboratory

Tetsu Tokunaga, Lawrence Berkeley National Laboratory

Thomas Torgerson, University of Connecticut

Donald Wyman Vasco, Lawrence Berkeley National Laboratory

Jiamin Wan, Lawrence Berkeley National Laboratory

David Wark, Rensselaer Polytechnic Institute

Alicia Wilson, University of South Carolina

Christopher D. White, Louisiana State University

Nicholas Woodward, Department of Energy

Xiaohui Xiao, Massachusetts Institute of Technology

Wenlu Zhu, Woods Hole Oceanographic Institution