SAND2013-3763C

Geosciences Symposium, 2013

Mark Taylor, mataylo@sandia.gov, Materials Reliability, 01442

High resolution Global Climate Modeling

Sandia has led an effort to develop a highly scalable atmospheric model for the NSF/DOE Community Earth System Model. Our model can make effective use of the hundreds of thousands of processors in DOE's leadership computing facilities, allowing us to run global climate simulations at weather resolving resolution. This increase in resolution is a key requirement for obtaining better assessments of regional climate change.

Timothy Draelos, tjdrael@sandia.gov, Next Generation Monitoring Systems, 05563

Probabilistic Event Detection and Signal Association

The Probabilistic Event Detection, Association, and Location (PEDAL) algorithm is an SNL-developed signal associator. It takes station detection observations of arrival time, azimuth, and horizontal slowness as inputs and outputs an event bulletin. PEDAL is designed to replace the current associator in use at international and national monitoring centers.

Scott Broome, stbroom@sandia.gov, Geomechanics, 06914

Source Physics Experiment Material Characterization

The Source Physics Experiment Program is conducted at the Nevada National Security Site and provides ground truth data to create and improve strong ground motion and seismic S-wave generation and propagation models; these upgraded models will provide improved detection of worldwide low yield nuclear testing activities. A key component in the predictive capability and ultimate validation of the models is the full understanding of the intervening geology between the source and the instrumented bore holes including the geomechanical behavior of the site rock/structural features. Three Source Physics Experiments have been conducted to date (a fourth is planned for Spring, 2013) and characterization work is in progress on material both pre shot and post shot.

Marissa Reno-Trujillo, mdreno@sandia.gov, Earth Systems Analysis, 06926

IMPACT-ing Policy Rather Than INFORM-ing Policy: Is it Possible?

After attending the American Water Resource Specialty Conference on Agricultural Hydrology and Water Quality last week and discussing what I heard there with Paul Kaplan, a Veteran Sandian, it has become disturbingly obvious to me that “sound science” is NOT reaching our policy-makers. For instance, in terms of our Ag-Food Critical Infrastructure, no matter how much good science there is to tell regulators that tile drains in the Corn Belt will lead to more intense flooding in the future, especially in the light of climate change that predicts a wetter Midwest, policies are unchanged and tile-drain salesman are making millions off of farmers who see only good in tile drains, which comes from their capacity to drain water-logged soils and enable higher corn yields to serve an increasingly profitable, greedy corn demand (50% for animal feed, 40% for ethanol, 9% to industry, 1% to humans). This is an incredible disaster on the verge of realizing itself. How do we change this?

Marianne Walck, mcwalck@sandia.gov, Geoscience, Climate, and Consequence Effects, 06900

Geo Research Foundation

The Geo Research Foundation is continuing its mission to build a bigger sense of community within the broadly dispersed people who do Geo and Atmospheric sciences research at Sandia. The presentation will extend awareness of the Foundation and continue dialog on how the Geo and Atmospheric community can have as much impact as possible as part of the Geo Research Foundation.

Kristopher Kuhlman, klkuhlm@sandia.gov , Repository Performance, 06212
Bwalya Malama, Jason Heath, Payton Gardner & Steve Bauer

Applying a hydrologist's tools to the problem of shale gas reservoir characterization

We are developing numerical and analytical solutions for fractured flow and multirate noble gas transport from dual-porosity low-permeability reservoirs, to be used in a Bayesian parameter estimation framework. Reservoir engineers tend to either use over-simplified models that don't correctly capture the physics of the problem, or they use a very complex numerical reservoir simulator, which they have no hope of ever parameterizing. Our proposed solutions will combine physically realistic rate transient analysis with multirate concentration decline curves for natural tracers.

Anastasia Ilgen, agilgen@sandia.gov, Geochemistry, 06915

REACTIVITY OF STRUCTURAL FE(II)/FE(III) COUPLE IN FE-RICH CLAY MINERALS

Redox transformations of nutrients and contaminants and their bioavailability in soils are controlled by heterogeneous chemistry on mineral surfaces. Structural iron Fe(II)/Fe(III) coupled in the octahedral sheet of clay minerals can directly participate in electron transfer reactions. We study the direction and kinetics of electron transfer using redox active elements - arsenic, selenium, chromium, and antimony - to probe the reactivity of clay structural iron under varying conditions.

Timothy Fuller, tjfulle@sandia.gov, Computational Structural Mechanics & Applications, 01525
Pania Newell

The Kayenta Material Model, Current Projects and Future Development Directions

The Kayenta geological material model is a three invariant cap plasticity model, available in SNL's Sierra SM, CTH, and Alegra finite element codes. Current applications of Kayenta range from blast of ceramic armor to flow in porous media. We'll discuss Kayenta's use in simulations involving porous flow in geologic media and solicit feedback for future development efforts.

Hongkyu Yoon, hyoon@sandia.gov, Geomechanics, 06914

Pore-scale investigation of single- and multi-phase flow, transport, and reaction

In many natural and engineering processes, fluid flow is often coupled with a variety of chemical reactions at the pore scale (e.g., nano- to micro-scales). In addition, the kinetics and mechanisms of water-mineral interactions are more complicated due to hydrodynamic processes in porous and fractured media. We currently cannot accurately model reactive transport behavior in geological formations due to both theoretical and observational disconnects between different fundamental scales (molecular, pore, laboratory, and field scales). Accurate prediction of coupled geophysical and chemical processes at the pore scale also requires realistic representation of pore structures. A series of lab experimental works involving mercury intrusion porosimetry, focused ion beam –SEM analysis (FIB-SEM), water imbibition experiments, diffusion, and pulse decay experiments can be integrated together to characterize multi-scale pore network structures and petrophysical properties. The image results can be used for pore-scale lattice-Boltzmann (LB) and/or direct numerical simulations in order to describe gas flow in pore structures at nano- to micron-scales, obtain permeability, relative permeability, and tortuosity at several different scales. Recent numerical and experimental efforts regarding carbon sequestration, shale gas flow, mineral precipitation and dissolution at the pore scale will be briefly presented. Upscaling this approach considered will also be discussed.

Ray Bambha, rpbambh@sandia.gov, Remote Sensing &Energetic Materials, 08128

Greenhouse gas source attribution for treaty verification

Current attribution approaches are unable to estimate greenhouse gas (GHG) fluxes with sufficient certainty for treaty verification or municipal decision support. We are deploying a mobile lab to measure abundances and fluxes of trace gases and particulates co-emitted with anthropogenic and biogenic GHGs. We are also developing the capability to perform inverse modeling studies to use these measurements and narrow the uncertainties on source characterization.

Marie Vernell Parkes, mvparke@sandia.gov, Geochemistry, 06915

Screening metal-organic frameworks for separation of oxygen

Coal-burning power plants are significant greenhouse gas emitters and a major source of pollutants; the pollution can be both reduced and more easily captured by burning an oxygen-enriched fuel. Metal-organic frameworks have recently emerged as excellent candidates for separating small molecules (including oxygen) from gas mixtures. With several thousand MOFs known, simulating adsorption isotherms using appropriate gas-MOF binding energies can help screen MOFs for specific separation applications.

Nedra Bonal, nbonal@sandia.gov, Geophysics & Atmospheric Sciences, 06913

Practical use of cosmic rays in the subsurface

I will be talking about the conclusions to my Early Career LDRD work on improving tunnel detection using seismic waves. I will also be talking about some proposed work using cosmic ray muons for imaging structures and the subsurface. Muons are passive source and nondestructive high-energy elementary particles that can travel relatively large distances making them ideal for this type of work.

Jang, Je-Hun; jjang@sandia.gov , Repository performance, 06212

Photon-induced regeneration of the simulated oxidized Fe solids

We observed that an Fe solid can reduce water to hydrogen by oxidizing itself. A few simulated oxidized Fe solids were synthesized. We are looking forward to electrochemically testing to see under what condition the simulated oxidized Fe solids can be regenerated by photon.

Ballard, Sanford[1], sballar@sandia.gov , Ground Based Monitoring, 05736
Michael L. Begnaud[2], Christopher J. Young[1], James R. Hipp[1], Andre V. Encarnacao[1] and W. Scott Phillips[2] , [1]Sandia National Laboratories and [2]Los Alamos National Laboratory

SALSA3D – A Global 3D P-Velocity Model of the Earth's Crust and Mantle for Improved Seismic Event Location

To test the hypothesis that high quality 3D Earth models will produce seismic event locations that are more accurate and more precise than currently used 1D and 2.5D models, we are developing a global 3D P wave velocity model of the Earth's crust and mantle using seismic tomography. We compare the travel-time prediction and location capabilities of our model to standard 1D and 2.5D models via location tests on a global event set with GT of 5 km or better. We obtain path-dependent travel time prediction uncertainties for our model by computing the full 3D model covariance matrix of our tomographic system and integrating the model slowness variance and covariance along paths of interest.

Megan Slinkard, meslink@sandia.gov, Ground –Based Monitoring R&E, 05736
Waveform Correlation

Waveform correlation is a whole new paradigm in seismic event detection. We use the fact that events from nearby locations tend to produce very similar traces at a station to detect, locate, and classify events more quickly and more accurately than with traditional methods. We've processed 3 years of central Asia data and found many events not included in global or regional catalogs.

Robert Abbott, reabbot@sandia.gov, Geophysics & Atmospheric Sciences, 06913

Development of a downhole, seven degree-of-freedom seismic instrument

Engineering of enhanced geothermal systems and recovery of unconventional hydrocarbon resources often require fracturing of the in situ rock. Determining the effectiveness of the fracturing and location of the fractures is an ongoing problem. Our project aims to create a superior downhole seismic tool for this purpose by combining 3 axes of translational sensors, three axes of rotational sensors, and a pressure sensor.

Paul Mariner, pmarine@sandia.gov, Applied Systems Analysis &Research 06224

Validation of atmospheric chemistry models hindered by biased rainwater pH data

Accurate atmospheric chemistry models are needed to understand and predict regional and global trends in composition and climate. One way to validate these models is to compare predictions of rainwater pH to national databases (e.g., NADP). This, however, is a problem when these pH data are biased (some too high by more than 2 pH units) due to the rapid microbial degradation of atmospheric organic acids in the collected rainwater samples.

Mathew Ingraham, mdingr@sandia.gov , Geomechanics, 06914

Intermediate Principal Stress Dependencies

Currently many of the models and theories developed for failure of geomaterials depends on the first and second invariants of stress (mean and shear stress essentially). However, work dating back to the early 60's shows that there is a dependence on the intermediate principal stress and therefore the third invariant of stress. To explore this phenomenon fully true triaxial tests are necessary, yet much of the work in the geological engineering field continues to ignore these critical failure parameters.

Hope Michelsen, hamiche@sandia.gov, Combustion Chemistry Dept., 08353

Effects of atmospheric black carbon on climate

Black carbon is strongly absorbing, contributes to climate change globally, and is believed to be a major contributor to Arctic warming, which is twice that of the global rate. We are building a field instrument (as part of the LDRD program) to measure atmospheric black carbon to reduce uncertainties in the understanding of its emissions, transport, aging, scavenging, and optical properties.

Kara Peterson, kjpeter@sandia.gov, Numerical Analysis & Applications, 01442

Predicting the Future Trajectory of Arctic Sea Ice: Reducing Uncertainty in Sea Ice Models

Our research is focused on the development of a systematic methodology to 1) evaluate predictive capabilities of sea ice models, 2) discover the most important physical parameters contributing to uncertainties and 3) assess the impact of numerical algorithms on sea ice simulations. For our evaluation we are using the LANL CICE code with two different rheological models that include a standard isotropic rheology and an anisotropic rheology that we have implemented.

Scott Lindblom, slindbl@sandia.gov, Geothermal, 06916
Ryan Hess 01716

High Temperature Chemical Sensing Tool for Enhanced Geothermal System Applications

The Geothermal Research Department (06916), in partnership with the Microsystems Enabled Detection Department (01716), is currently developing a high temperature downhole chemical sensing tool. This tool will be used to measure the in-situ concentration of ionic tracers commonly deployed for characterizing fractures in enhanced geothermal systems. While a species of interest has not been selected for the prototype tool, development and testing is underway on novel high temperature electrodes to detect Li, Cs, Br and I as well as pH.

Edward Matteo, enmatte@sandia.gov , Nuclear Waste Disposal Research & Analysis 06222
Tom Dewers, Steve Bauer, Alex Urquhart (UNM), John Stormont (PD/PI, UNM), Mahmoud Taha (UNM), Andrew Duguid (Schlumberger)

Wellbore Seal Repair using Nanocomposite Materials

The DOE-NETL funded project, *Wellbore Seal Repair using Nanocomposite Materials*, is a 3 year project (FY13-FY15) that aims to produce cementitious nanocomposite materials to be used to repair "leaky" wellbores that intersect a subsurface carbon dioxide storage reservoir. Ensuring the seal integrity of abandoned wellbores is critical to ensuring permanent containment within a carbon dioxide storage formation. Since thousands of abandoned wellbores may lie within the aerial extent of a typical carbon sequestration operation, repairing damaged wellbores is potentially an economically attractive alternative to the relatively expensive operation of well re-completion. SNL is lending its expertise in both wellbore integrity and carbon sequestration to this project that includes collaborators from the University of New Mexico and industry.

Elena Kalinina, eakalin@sandia.gov , Storage & Transportation Technology, 06225
Tom Lowry, Kate Klise, and Teklu Hadgu

Reducing Uncertainty in Enhanced Geothermal System (EGS) Development.

The Enhanced Geothermal Systems (EGS) have great potential for producing clean and reliable energy. As of today, the EGS are in the stage of development with a few demonstration projects in place around the world. The existing difficulties with the EGS and the large capital investments required to start such a project make this type of geothermal energy unattractive for industries and uncompetitive with other forms of renewable energy. The goal of our project is to address this problem by reducing the risks involved in developing geothermal resources. We use multi-scale, multi-model approach that consists of high-resolution heat and transport simulations and systems level analysis. To represent the EGS reservoir conditions in heat and transport simulations we developed a Fractured Continuum Model (FCM) that incorporates fully three-dimensional representations of anisotropic permeability, multiple independent fracture sets, and arbitrary fracture dips and orientations. The reservoir model allows for evaluating the impacts of different EGS conditions on heat extraction and for comparing alternative heat extraction schemes. The systems analysis model is used to assess the tradeoffs between the costs of developing the various scenarios, and the potential economic return on the power production.

Oksana Guba NMN Materials Reliability, 01442

Development of the spectral element dynamical core in the Community Atmosphere Model

We describe the spectral element dycore in the Community Atmosphere Model. We give an overview of the dycore's scalability and conservation properties. Also, we present recent developments for the advection scheme, stabilization techniques, and for simulations with variable resolutions.