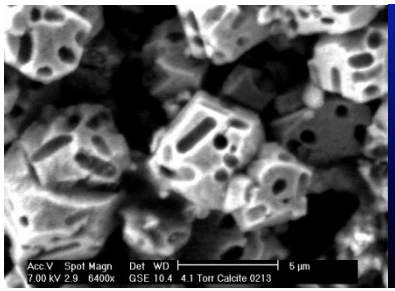
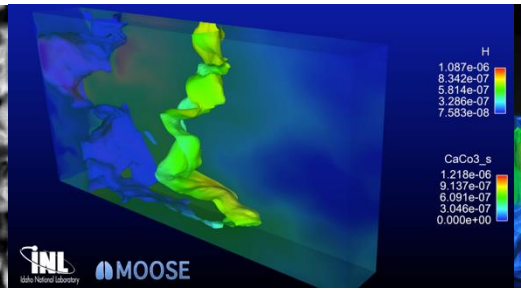
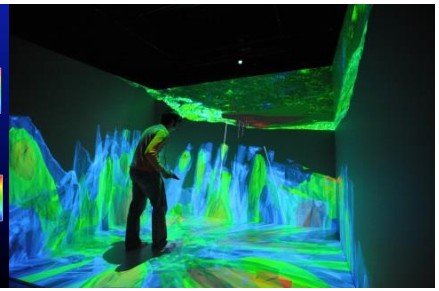
Discover, Demonstrate, and Secure Innovative Nuclear, Clean Energy, and Environmental Solutions At-Scale, and Protecting our Critical Infrastructure







Kelly Beierschmitt, Ph.D.
Deputy Lab Director-Science and Technology
Chief Research Officer

BERAC Meeting

March 2016

www.inl.gov

Idaho National Laboratory

Environmental Subsurface Science - Complemented by Nuclear and Radiochemistry

Fundamental studies to applications, molecular-scale to industry-scale

Subsurface Fate and Transport

- Biogeochemistry
  - Radionuclide interactions
  - Isotope ratios
- Characterization
- Reactive transport modeling

Next Generation Subsurface Energy Systems

- Fracturing
- Innovative sensing
- Ultrasensitive detection of radionuclides
- Advanced multiphysics, multidomain simulation framework

System Integration, Validation And Verification

- System dynamics
- Decision analysis
- Risk-based assessment

New Technologies & Processes for:

- Remediation of radionuclide contamination
- Geothermal energy production
- Geologic storage of nuclear waste
- Combined recovery of unconventional fossil fuels from and CO_2 sequestration in nanoporous shale

INL core capabilities to tackle compelling S&T challenges

Advanced Computer Science, Visualization, and Data
Applied Materials Science and Engineering
Biological and Bioprocess Engineering
Chemical and Molecular Science**
Chemical Engineering
Condensed Matter Physics and Materials Science**
Cyber and Information Sciences
Decision Science and Analysis

Environmental Subsurface
Large-Scale User Facilities/Advanced Instrumentation
Mechanical Design and Engineering
Nuclear and Radio Chemistry
Nuclear Engineering
Power Systems and Electrical Engineering
Systems Engineering and Electrical Engineering

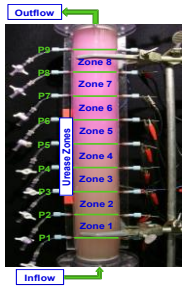
People: 160, Postdocs:4;
Copyright, Patentable IP: 8;
Programs: DOE (NE, EM, FE, EERE), DOD, EPA

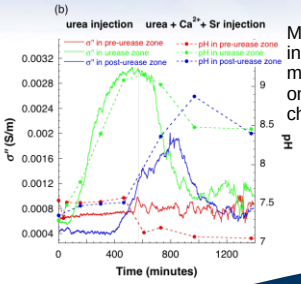
Fujita, Y. et al. (2010), Evaluating the potential of native ureolytic microbes to remediate a ^{90}Sr contaminated environment. *Environmental Science &Technology*, 44, 7652-7658, doi: 10.1021/es101752p.
Huang, H. et al. (2005), Modeling of multiphase fluid motion in fracture intersections and fracture networks, *Geophysical Research Letters*, 32, L19402, doi: 10.1029/2005GL023899.
Guo, L. et al. (2013), A parallel fully-coupled fully-implicit solution to reactive transport in porous media using preconditioned Jacobian-free Newton-Krylov method, *Advances in Water Resources*, 53, 101-108, doi: 10.1016/j.advwatres.2012.10.010.
Snyder, D. C. et al. (2012), Radioactive cesium isotope ratios as a tool for determining dispersal and re-dispersal mechanisms downwind from the Nevada Nuclear Security Site, *Journal of Environmental Radioactivity*, 110, 46-52, doi: 10.1016/j.jenvrad.2012.01.019.

Integrate Fundamental Science into Unifying Predictive Computational Framework Enabling End-Use Applications

Idaho National Laboratory

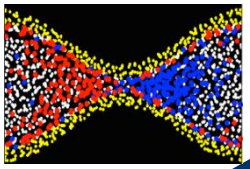
Adaptive monitoring of processes and property changes in complex environments





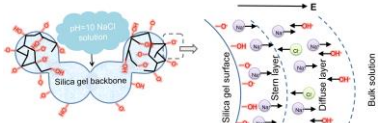
Macroscopic spectral induced polarization measurements detecting onset and location of chemical changes

Dissipative particle dynamics Simulation of induced Polarization near pore throat



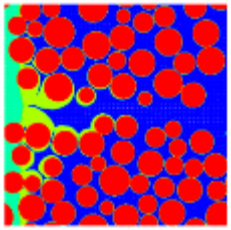
Development of unifying computational frameworks and interoperable models for linking the subsurface environment and terrestrial ecosystems.

Continuum/field scale



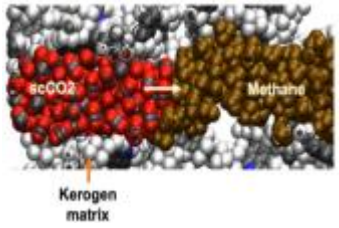
Electrical double Layer (EDL) model

Pore-scale coupled processes

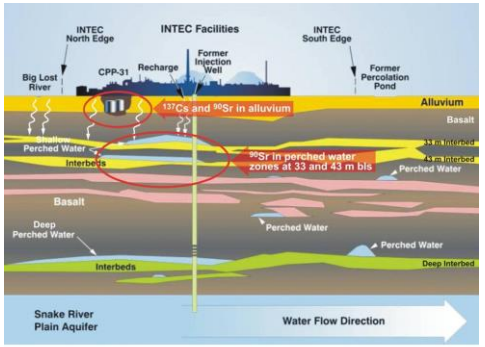


Pore clogging due to mineral precipitation

Molecular and nanoscale processes



Predictive understanding of coupling between (bio)geochemical processes and material property changes across spatial and temporal scales



Conceptual model of contaminant distribution and transport in deep fractured vadose zone at INL site

Increase FTEs and postdocs; FY 20: > $20M; Additional programs: DOE (BER, EM, ASCR, BES, EERE), Industry

Integrated Experiments & Physics-Based Modeling of Contaminant Fate & Transport in Deep Fractured Vadose Zone

Core facility - Geocentrifuge (2m radius, 50 g-ton capacity) enables unsaturated flo w experiments

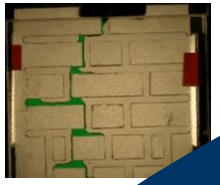
Core facility - State of the art chemical, biological, materials characterization laboratories; HPC facilities

Bench-scale analog fracture network

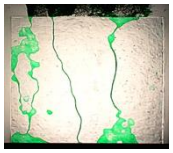
100m diameter infiltration test at INL

Core facility - Vadose Zone Research Park and other field test capabilities

~cm scale analog fracture network



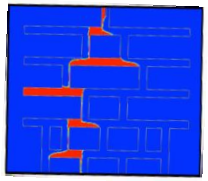
Intermittent flow in single fracture – geocentrifuge experiment



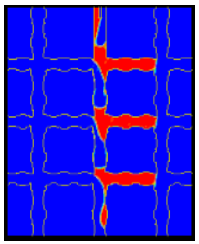
Field

Intermediate: ~m

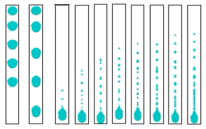
Hele-Shaw cell: ~cm



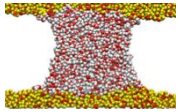
Simulation of flow focusing



Gravity-driven avalanching & cascading

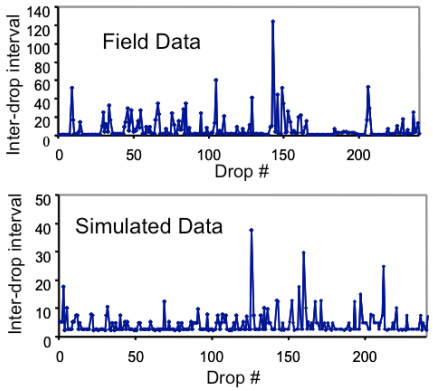


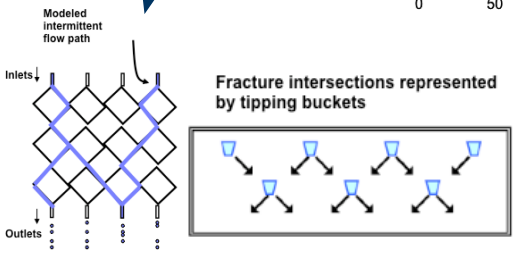
Periodicity, bifurcation and chaos of droplet flow in single fracture



MD – contact line dynamics

Episodic flow observed in field experiment and numerical model





Next generation stochastic model for fractured vadose zones

Conventional unsaturated flow theory breaks down in fractured vadose zone!

Key references:

Wood, T. and H. Huang (2015), Fluid Dynamics in Complex Fractured-Porous Systems (AGU Geophysical Monograph Series) 210: 209.

Huang, H. and P. Meakin (2008), *Water Resources Research*, 44, W03411, doi: 10.1029/2007WR006158.

Liu, M. et al. (2006), *Physics of Fluids*, 18, 017101, doi: 10.1063/1.2163366.

Huang, H. et al. (2005), *Geophysical Research Letters*, 32, L19402, doi: 10.1029/2005GL023899.

LaViolette, R.A. et al. (2003), *Geophysical Research Letters*, 30(2), 1083, doi: 10.1029/2002GL015775.

Huang, H. at al. (2005), *Water Resources Research*, 41, W12413, doi: 10.1029/2005WR004204.

Wood, T. R. et al. (2002), *Geophysical Research Letters*, 29(24), 2191, doi: 1029/2002GL015551.

Partnerships to Accelerate Outcomes, Deliver Innovation & Impacts, and Develop Next Generation Scientists & Engineers

Microscopy and Characterization Suite, unique capabilities for working with irradiated and radioactive materials.

Imaging and tomography of nano- and sub-nanoscale microstructure of geomaterials; In situ measurements and imaging of nanosecond-scale dynamic processes; Fluid/fluid/solid interface molecular dynamics modeling and quantum chemistry calculations.

Fate & transport in porous media; thermodynamics of fluids in confined nanopores; geomechanics and fracturing driven by chemical/hydraulic/thermal perturbations

Idaho National Laboratory