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Community Software: Sierra Capabilities for Coupled Reactive Flow and Mechanics in Porous Media

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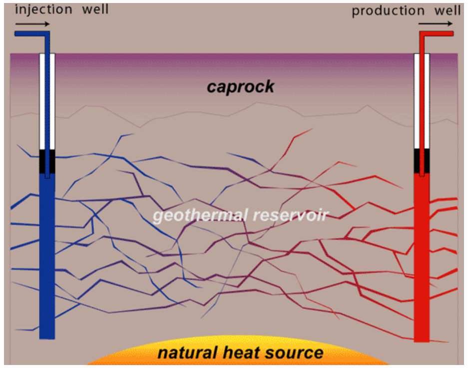
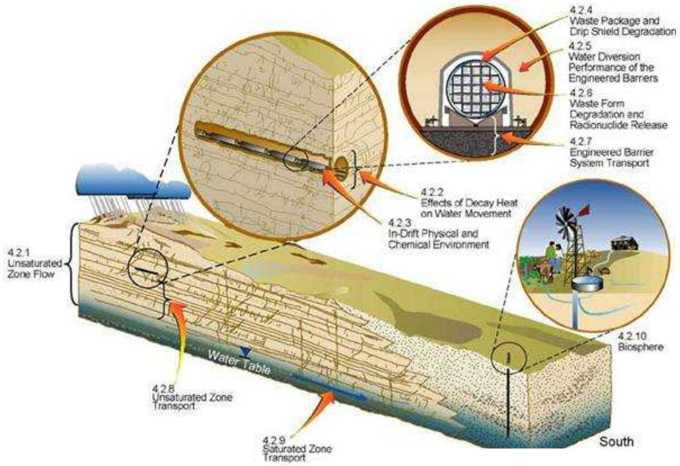
Geoscience Applications at SNL

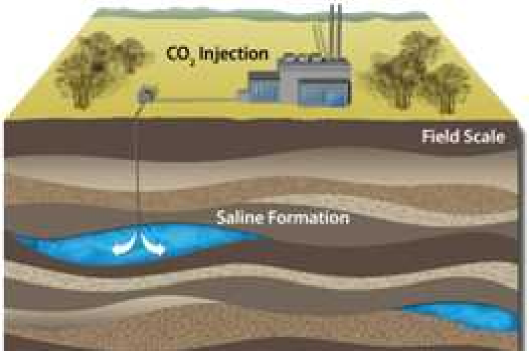
Engineered Geothermal



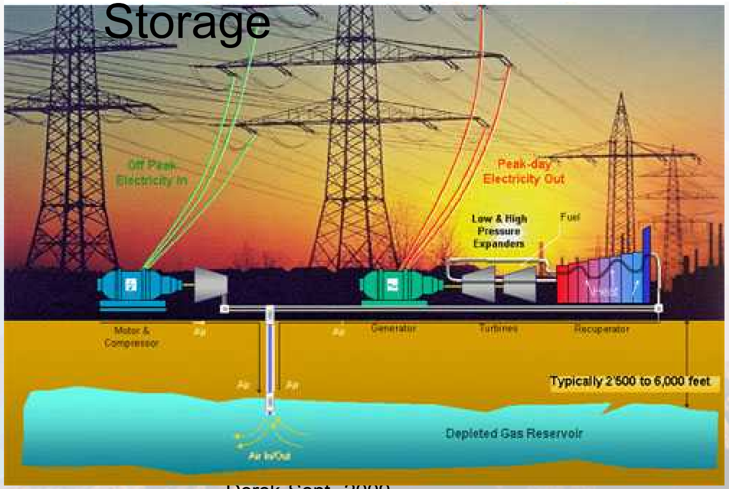
Nuclear Waste Isolation



CO_2 Sequestration

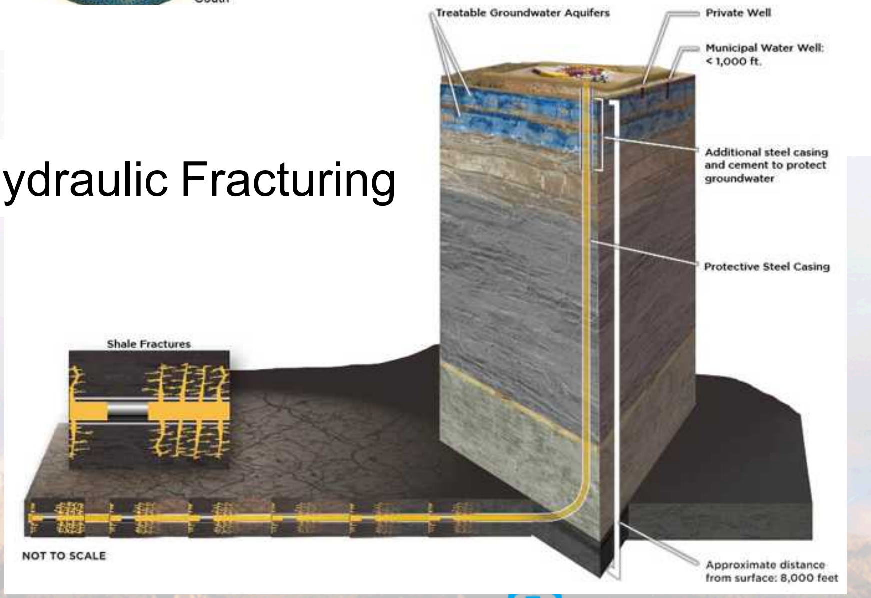


Compressed Air Energy Storage



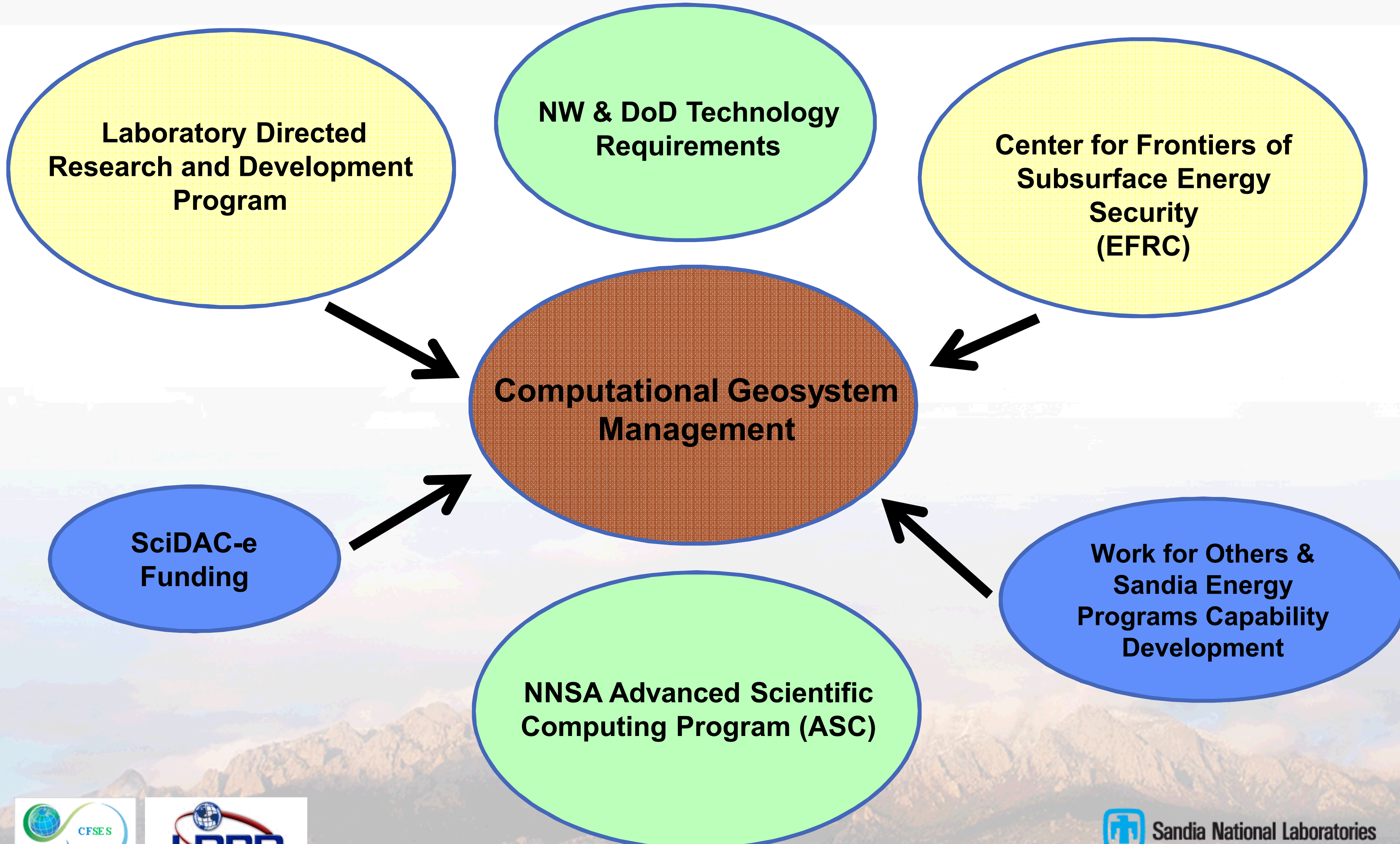
Derek Sept. 2009

Hydraulic Fracturing



http://www.hydraulicfracturing.com

Sandia Computational Geoscience Research and Subsurface Management Program



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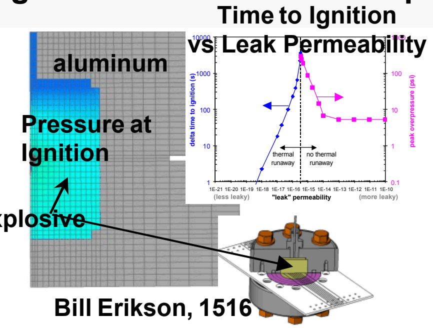
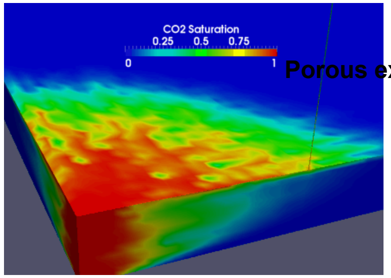
Overview of Porous Flow in Aria

- **Leveraged development under LDRD & EFRC**
  - Targets SNL activities in energy security, conventional munitions, thermal batteries, heat pipes, …
- **Current capabilities**
  - Single phase heat and reactive mass flow
  - Immiscible two-phase flow
  - Two-phase, two-component (air & water) evaporating/condensing thermal model
  - Chemically reactive flows (e.g. calcite mineralization)
  - Spatially heterogeneous material and transport properties
  - Couples with mechanics and other Sierra physics modules
- **Capability under development**
  - Nonisothermal two-phase CO2-H2O-NACL EOS with general phase behavior
  - Advanced discretization schemes (UT technology)

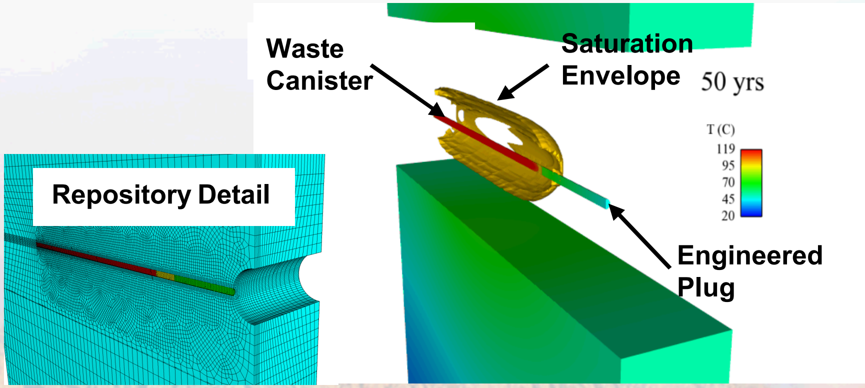
Modeling Cook-Off in Granular Explosives





CO_2 saturation levels in a brine-filled reservoir represented with uncorrelated heterogeneous permeability

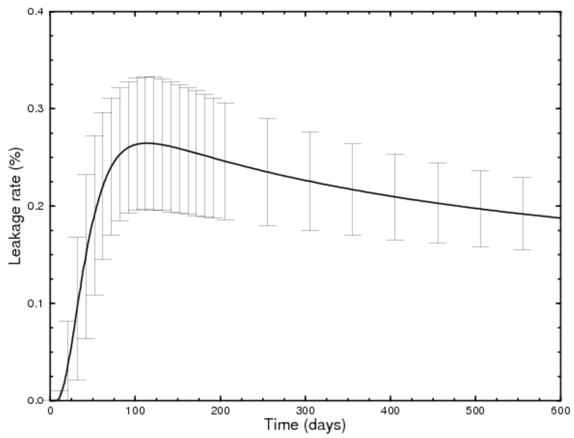
Heat-Generating Waste Disposal



Development of a confining saturation envelope in ultra-low permeability clays, trapping gases within.

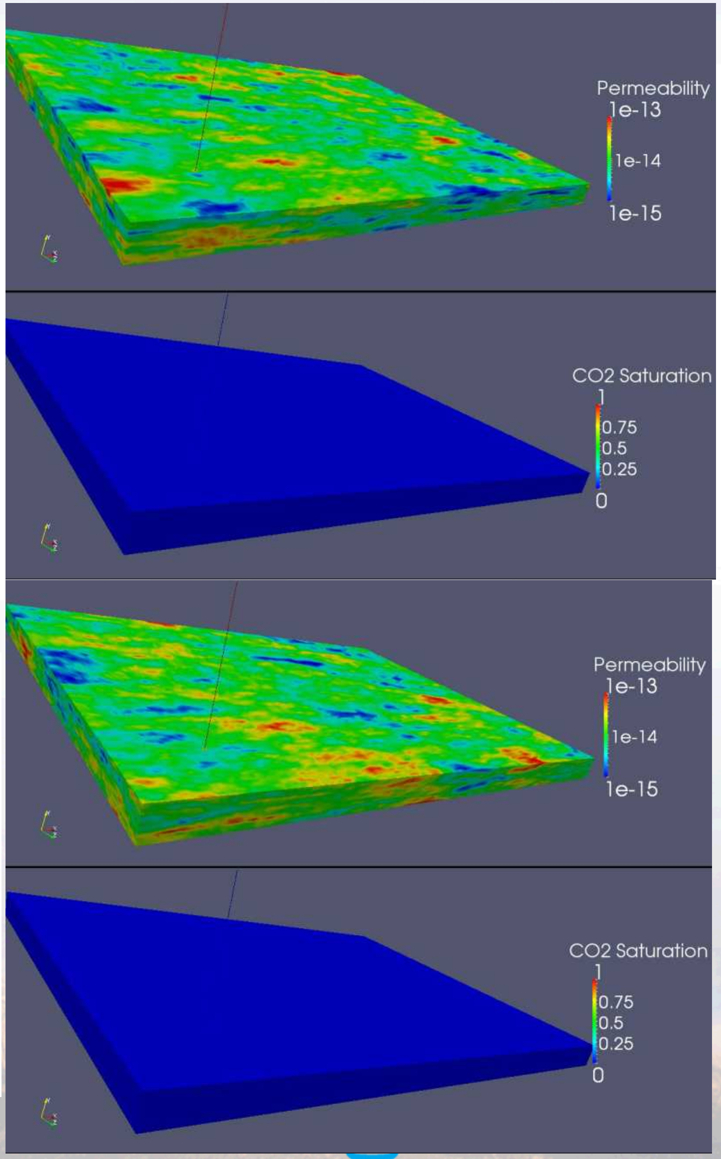
CO2 Leakage Through an Abandoned Well
Effects of Heterogeneity

Average Leakage Rate and Std. Dev.

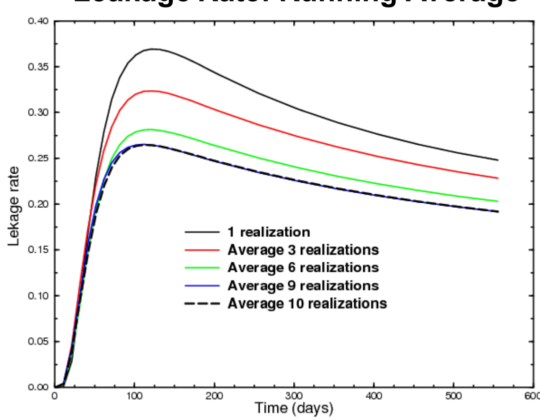


Some Results
(10 realizations)

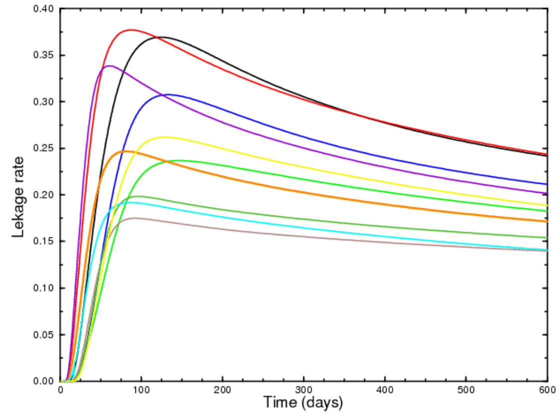
- Correlation between fast paths and permeability distribution is evident
- Leakage, arrival time are heavily dependent on permeability distribution
- Standard deviations are substantial
- Appears useful results can be obtained from a few realizations



Leakage Rate: Running Average

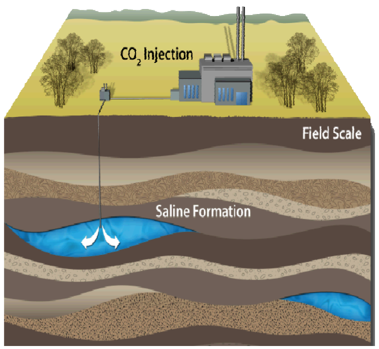


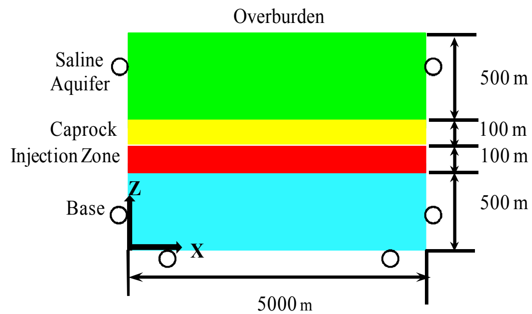
Leakage Curves



Coupled Flow and Geomechanics

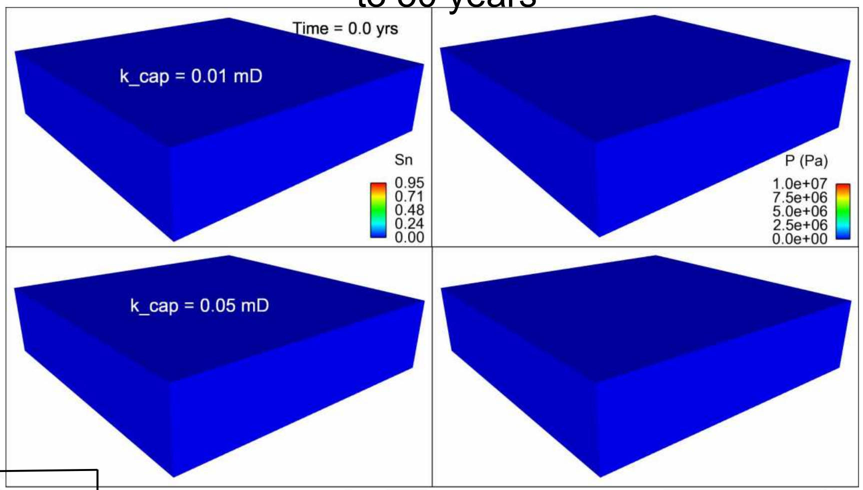
Flow, CO2 Transport and Deformation

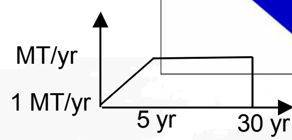


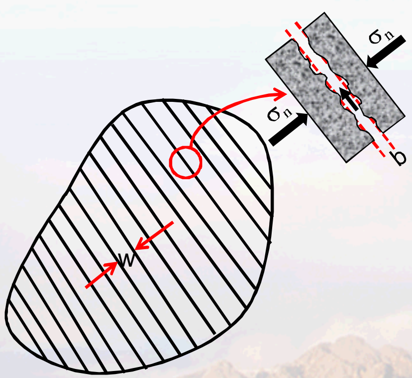


Model problem definition showing conceptual stratigraphy (left), and model problem geometry (right, not to scale).

CO_2 saturation, Overpressure & Displacement to 50 years

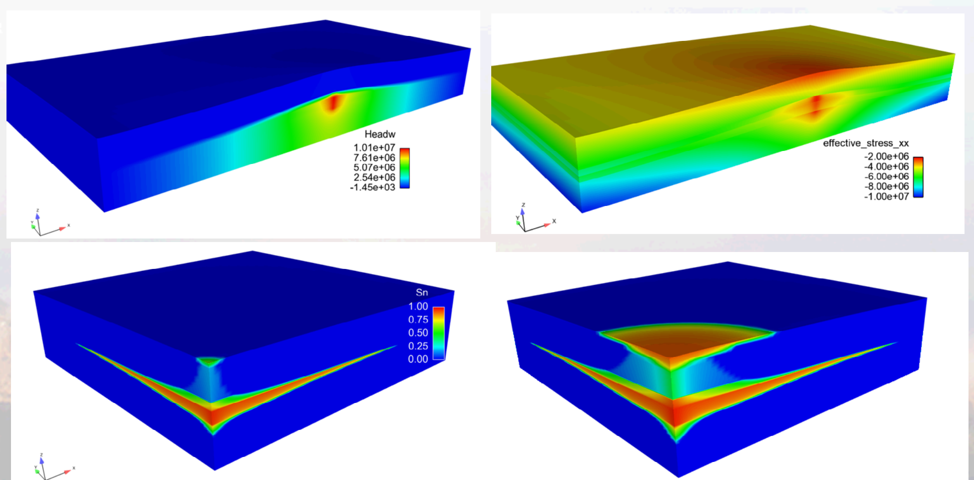






Conceptual Model for Jointed Rock

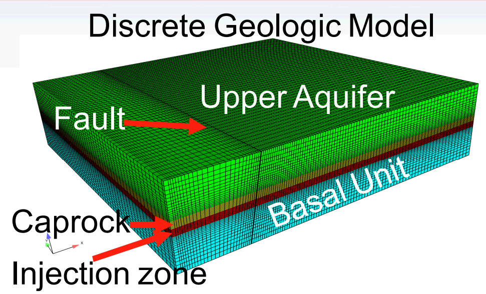
CO_2 Leakage in Jointed Rock



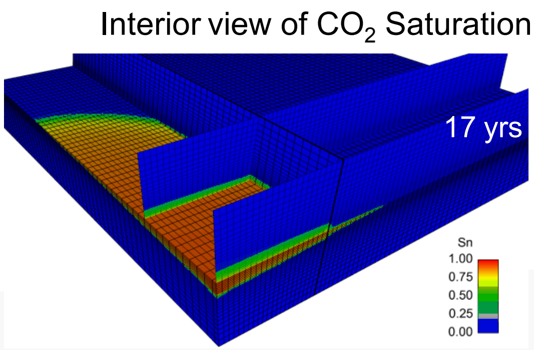
Coupled Flow and Geomechanics

Hydromechanical Effects of Faults

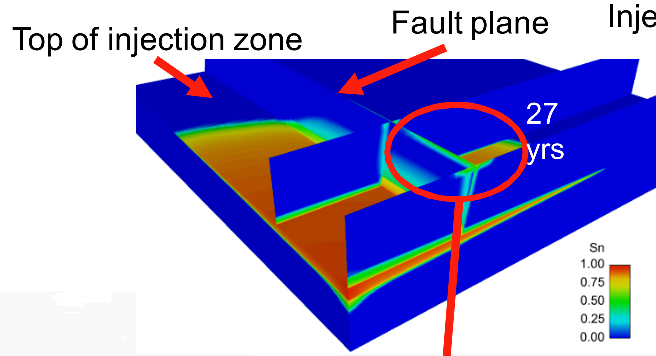
Some faults could go undetected and may pose a risk to sequestration of CO_2 by reactivation due to injection pressures. This study considers possible hydromechanical effects due to a low and high permeability fault.

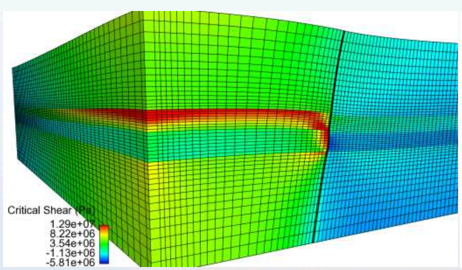


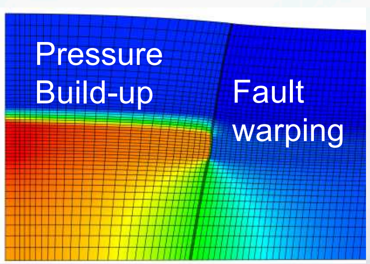
Low Permeability Fault

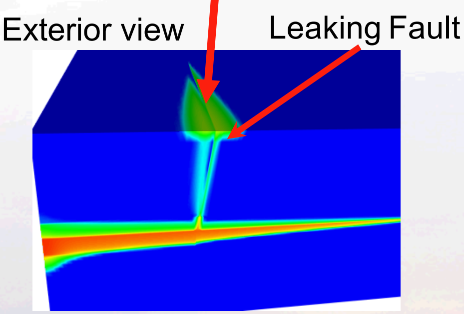


High Permeability Fault









Low permeability fault impedes CO_2 injection, diverts flow along fault and builds pressure behind the fault, thereby shearing/warping the fault and inducing critical shear failure in both the caprock and fault.

High permeability fault creates a pathway for leakage of CO_2 through the caprock, ultimately pooling at the top of the upper aquifer, which is capped by an impermeable boundary.

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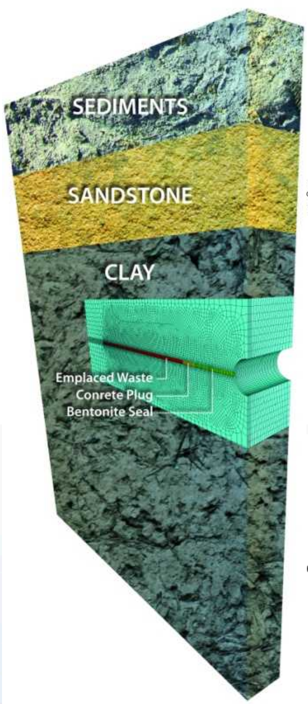
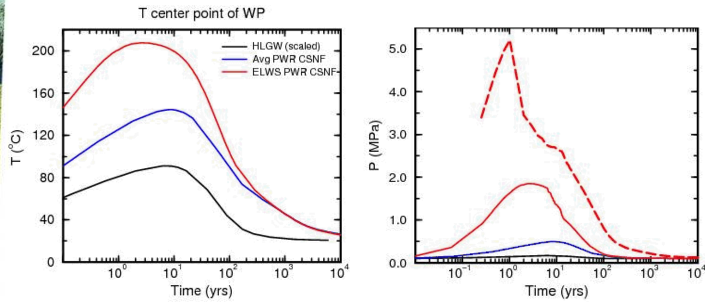
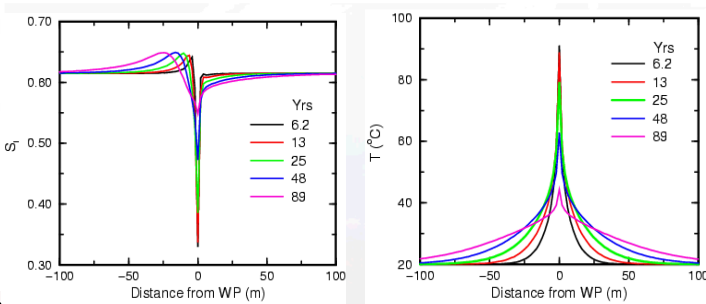
High Level Waste Disposal in Clay
Thermo-Hydrologic Features



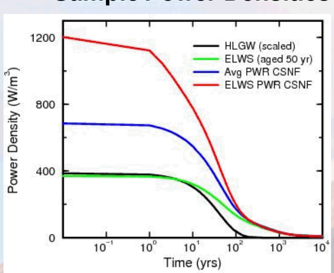
Repository Temperature and Pressure



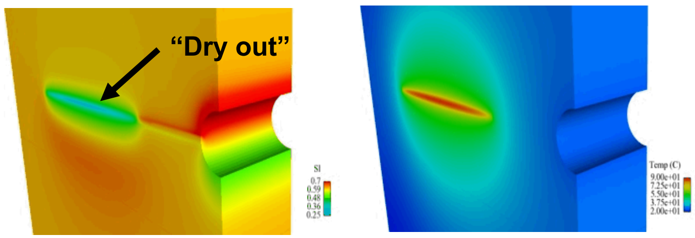
Spatial Variation of Temperature and Pressure

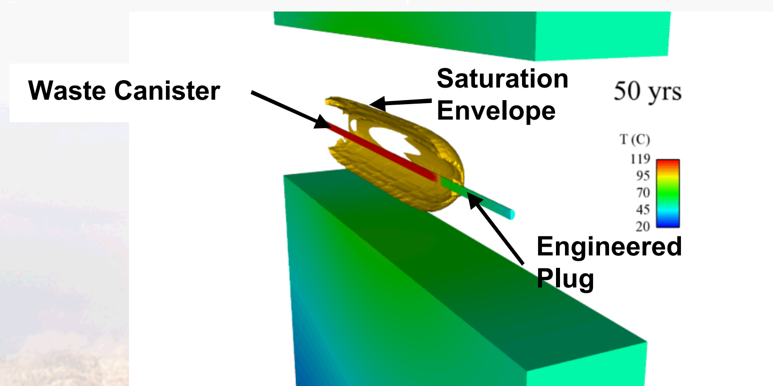


Sample Power Densities



High decay powers in ultra-low permeability clays can result in dry out regions and saturation envelopes.





Development of a confining saturation envelope in ultra-low permeability clays, trapping gases within.

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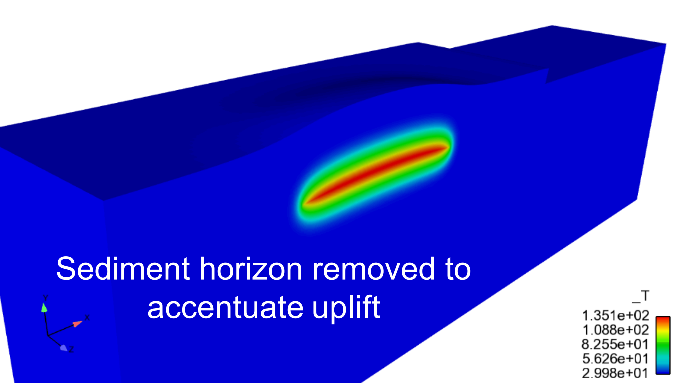
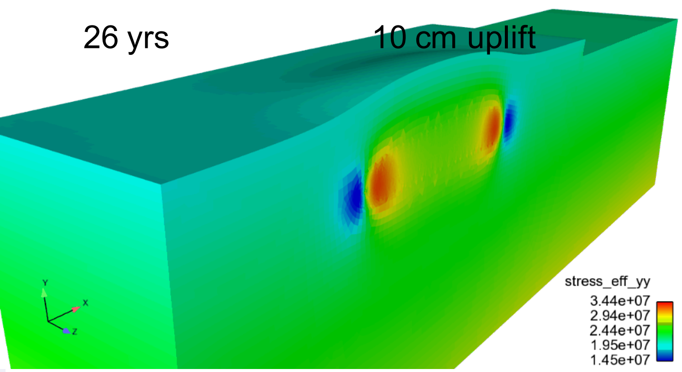
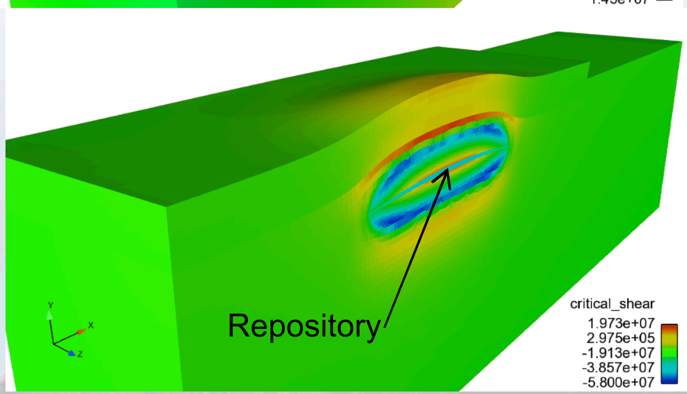
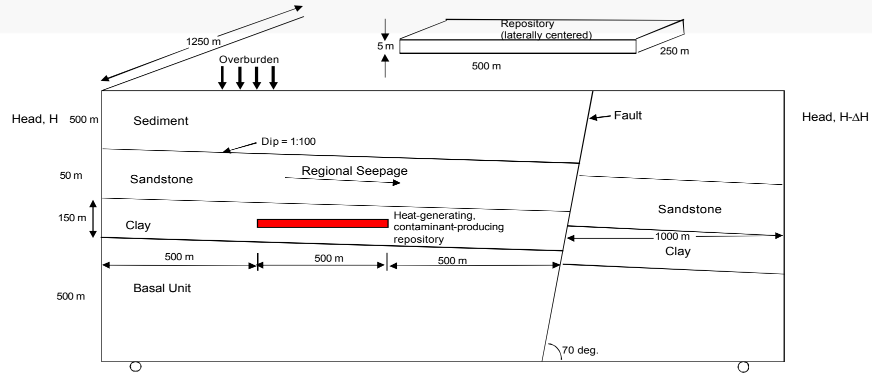
Coupled Energy, Flow, Radioactive Species, and Mechanics of a Clay/Shale Repository





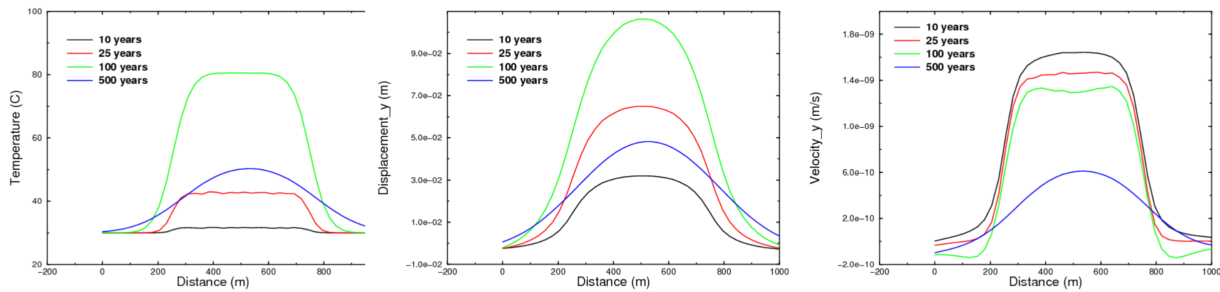


Problem Schematic



Thermal Expansion

- Localized deformation near repository
- Large stress gradient at the ends of repository
- Shear failure in clay/shale above and below repository, but not in "soft" repository



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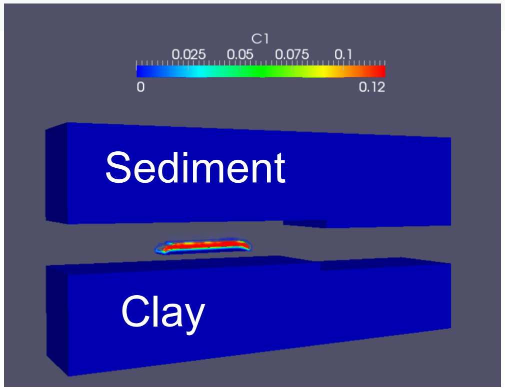
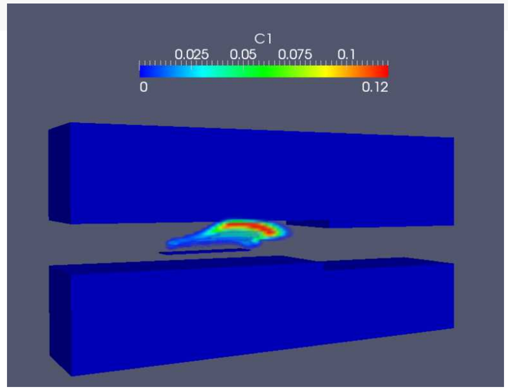
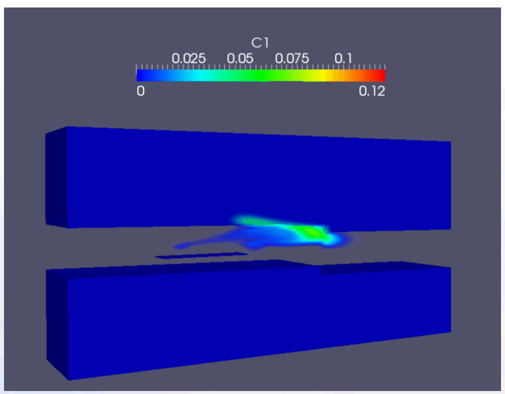
Transport of Daughter Species



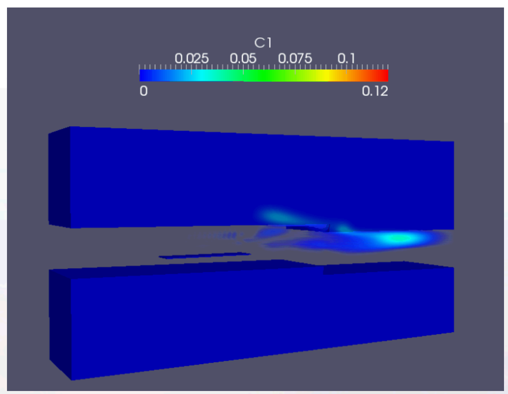
100 yrs



500 yrs



1000 yrs



2000 yrs

Sandstone & repository horizon removed to accentuate contaminant plume

Radioactive Decay Chain:

$$\frac{DC_0}{Dt} = -\lambda_0 C_0$$

$$\frac{DC_1}{Dt} = +\lambda_0 C_0 - \lambda_1 C_1$$

Half-Life (yrs):

C_0: 100

C_1: 10,000

Features:

- C_0 disappears early
- C_1:
  - rises to high-flow sandstone layer
  - rapid transport out of domain
  - some is trapped in sediment

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Pore Scale Analysis of Reaction Dependent Viscosity Variations for Subsurface Engineered Systems

Scientific Achievement

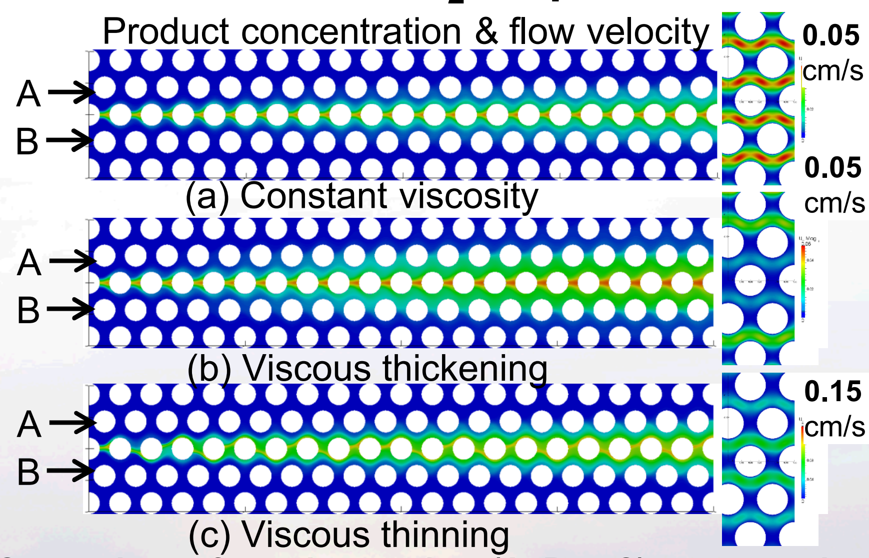
Developed a computationally powerful & highly parallelized pore-scale model to examine flow in porous media with chemical reaction dependent viscosity

Significance and Impact

Pore scale simulations on high performance computers suggest that mixing-induced chemical reactions can alter fluid properties (e.g., viscosity and density) and shear rate enabling engineered solutions for CO_2 sequestration

Research Details

- More reaction product was formed when fluid viscosity increases with increasing product concentration (viscous thickening) than the opposite case (viscous thinning)
- Enhanced mixing at pore scale leads to enhanced reaction rates at high local ratio of reaction rate to flowrate (Da) and lower porosity
- Flows with viscous thinning reactions can become unstable at high Da, leading to enhanced mixing and reaction rates under high Peclet number and higher porosity



Comparison of reaction product (A+B -> C) concentration and flow velocity in the loosely packed array for different viscosity variations. Hot (or cool) color depicts high (or low) concentration and velocity. Onset of Instability is shown in (c).

S.M. Davison, H. Yoon, and M.J. Martinez, Advances in Water Resources, 38, 70-80 (2012)

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