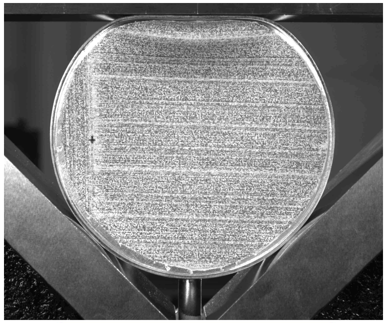
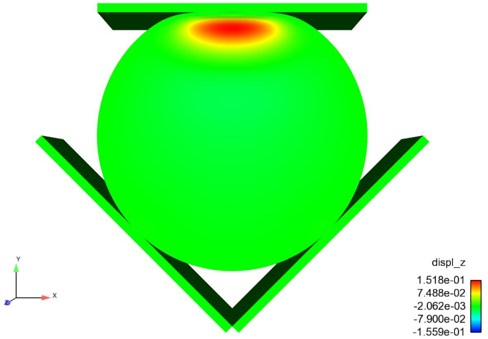
SAND2016-0731PE

Two Essential Aspects of Solid Mechanics: Material Modeling and Computational Mechanics





Pania Newell

Sandia National Laboratories

Exceptional service in the national interest

Presented to

The Department of Mechanical Engineering

University of Utah

January 25, 2014

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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MATERIAL MODELING AND CHARACTERIZATION

Motivation and objectives

- Almost every aspect of modern life involves **materials** and benefits from advances in **materials modelling**.
- Many of our challenging problems, such as climate change, energy production and healthcare, etc. require methods for probing the properties over a wide range of materials.
- **Materials modelling** can be used to solve real issues and problems and push cutting edge research.
- Used in combination with good analysis and experimentation, **materials modelling** can drive progress, saving time, effort and resource.

Constitutive modeling

- Mathematical formulation describing material respond to various loading.
- The *constitutive model* for a material is a set of equations describing the relationship between stress and strain (and possibly strain history, strain rate, and other field quantities).
- Some examples:
  - Plastically bonded explosive material
  - **Sandy Soil**
  - Mount Simon Sandstone
  - Laser weld
  - Polymer liked material (PEEK)

Constitutive modeling in geomaterial

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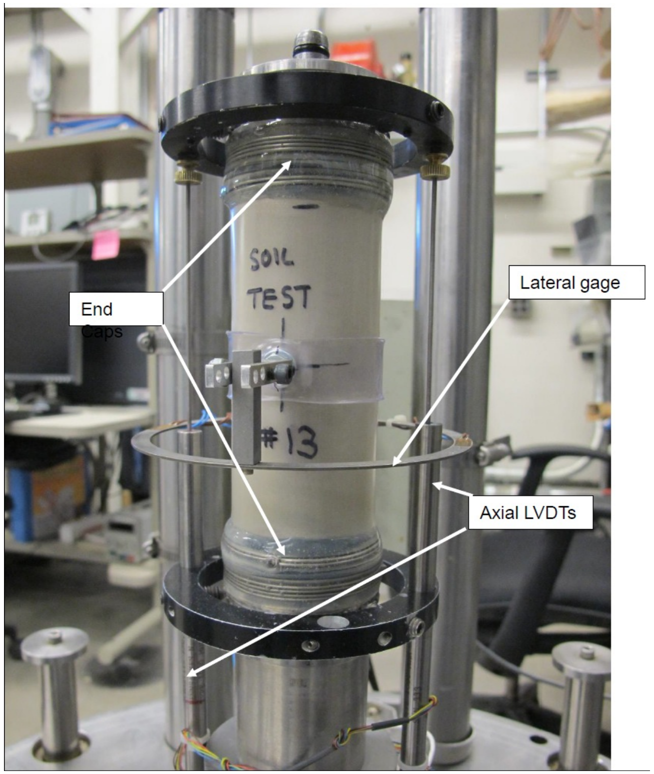
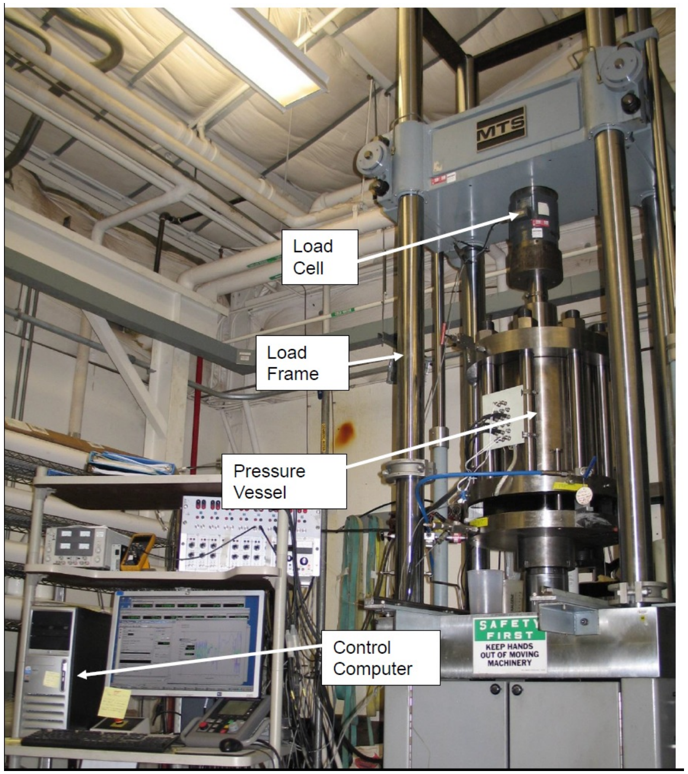
- Using the same mathematical plasticity theory for metals **NO**
- The constitutive behavior of geomaterials are different from that of metals in four distinct ways:
  - Geomaterials are highly compressible (pressure-volume response).
  - Geomaterial's yield strength depends on the mean stress.
  - Geomaterial's yield strength depends on the relative magnitudes of the principle stresses (third stress invariant).
  - Geomaterial's tensile strengths are much smaller compared to their compressive strengths.
- Unlike metals, whose constitutive bahavior can be characterized with only uniaxial tests, geomaterial characterization requires a *suite of material testing.*

Experimental testing design

A series of UCS, ASC, hydrostatic, and uniaxial strain experiments were conducted at Sandia's Geomechanics Laboratory.



Instrumented sample mounted on the 100 MPa pressure vessel base.

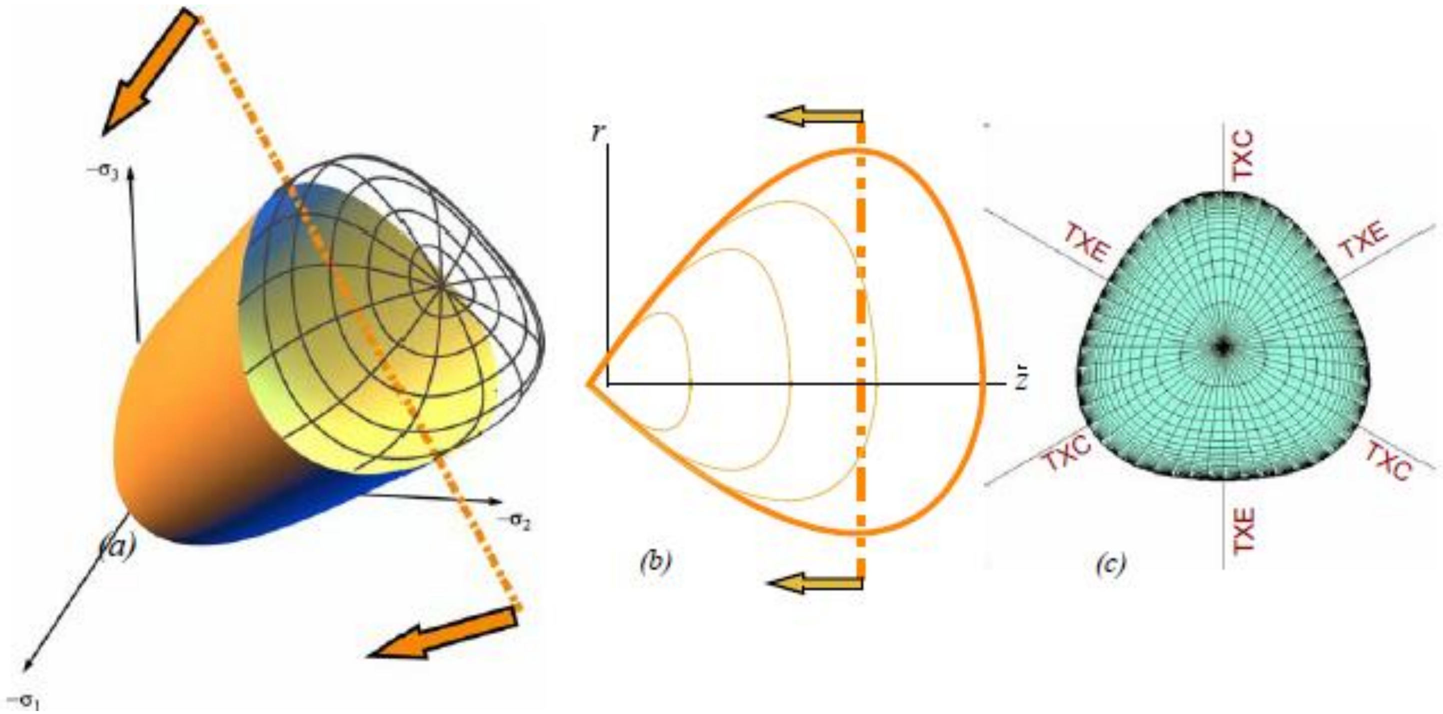


220,000 lb (1 MN) load frame with 15,000 psi (100 MPa) pressure vessel. Data acquisition system is show to the left of the load frame.

Constitutive modeling

- Observed elastic-plastic behavior from testing
- Decided to apply *Kanyenta* a generlized plasticity model developed by Prof. Brannon.
- Some of Kayenta's unique features:
  - Three-invariant, mixed hardening, non-associative plasticity.
  - Nonlinear (stress dependent) elasticity.
  - Nonlinear peak shear failure threshold for fully damaged material.
  - Kinematic hardening.
  - Nonlinear compaction function (pressure-volume) with isotropic hardening.

Kayenta material model



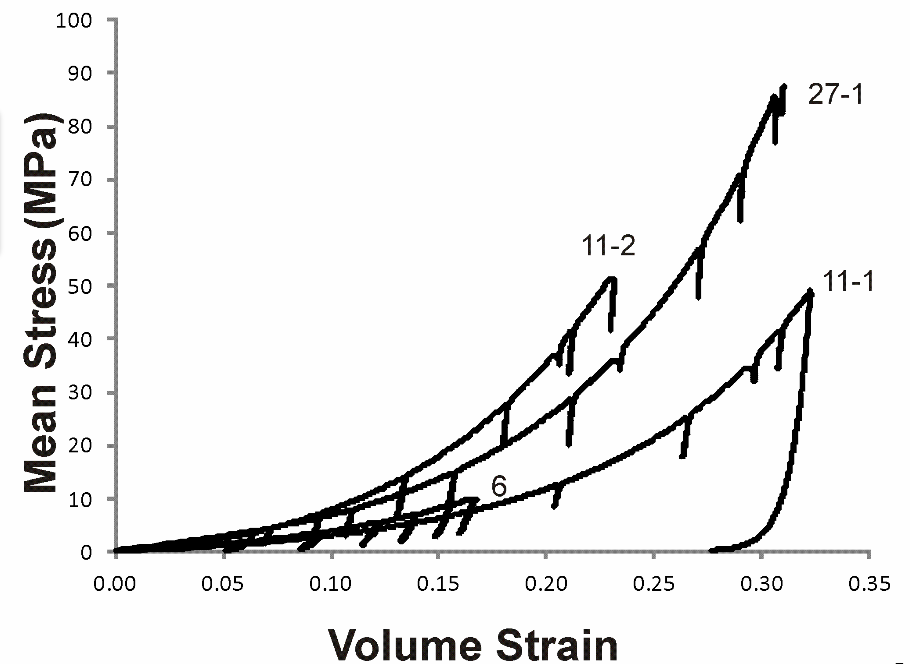
- Kayenta continuous yield surface
  - (a) 3D view: Principal stress space with the high pressure “cap”
  - (b) Side view: Using cylindrical coordinate system
  - (c) The Octahedral view: Looking down at the hydro stat

Brannon et al., 2009

Bulk and shear modulus

- Initial loading up to yield, and unloading curves for all load paths display a *nonlinear elastic* behavior.
- With an assumption of isotropy, these can be quantified by a stress-dependent bulk and shear modulus.
- Bulk modulus:

$$K = K_0\left(1 + K_1\sigma - K_2\exp^{-K_3\sigma}\right)$$



Shear modulus

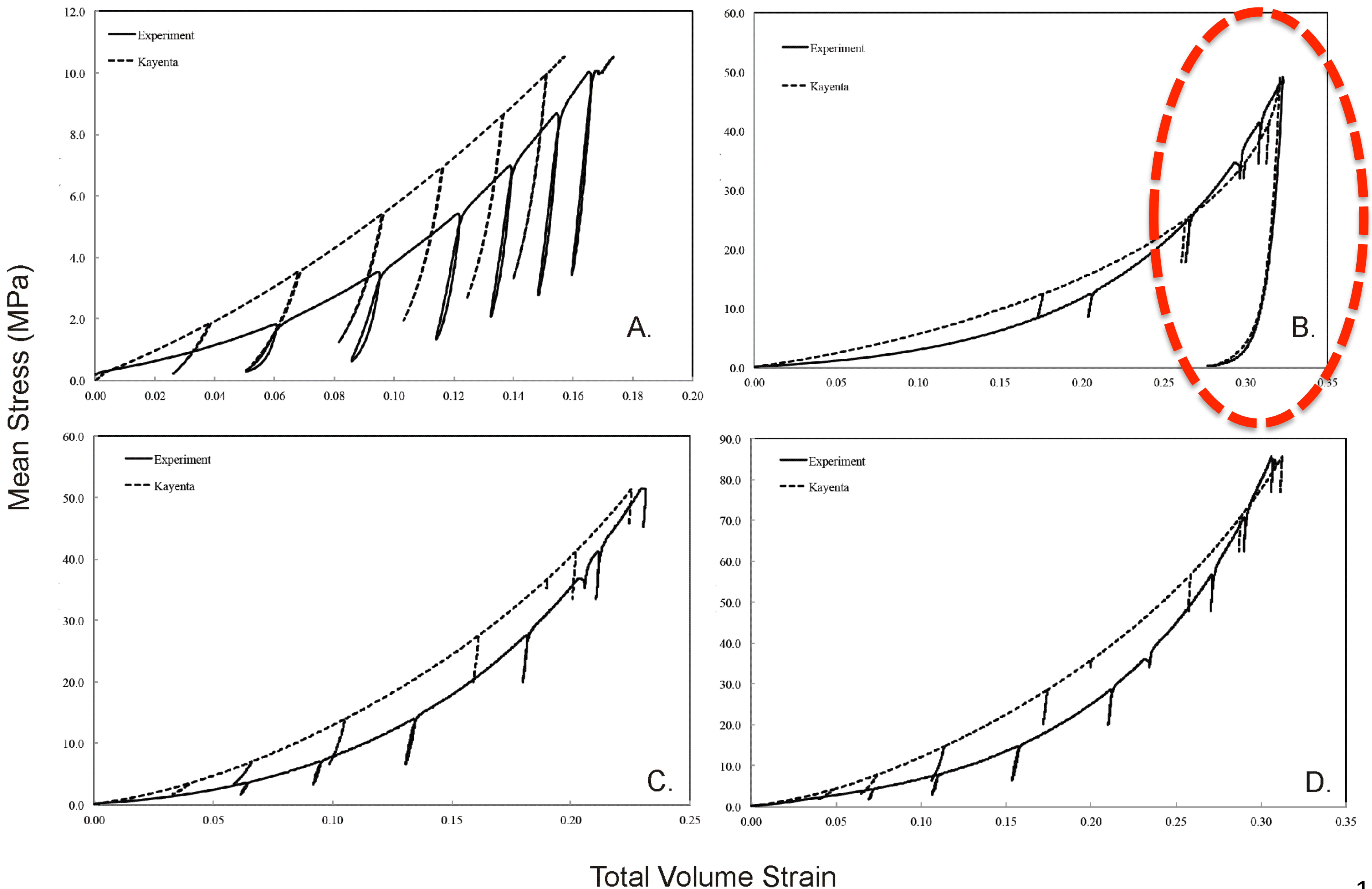
- In the case of uniaxial and non-hydrostatic portions of the triaxial tests, the axial stress-strain data was used to determine the Young's Modulus, E, and then find the shear modulus from the following expression:

$$E = \frac{9KG}{3K + G}$$

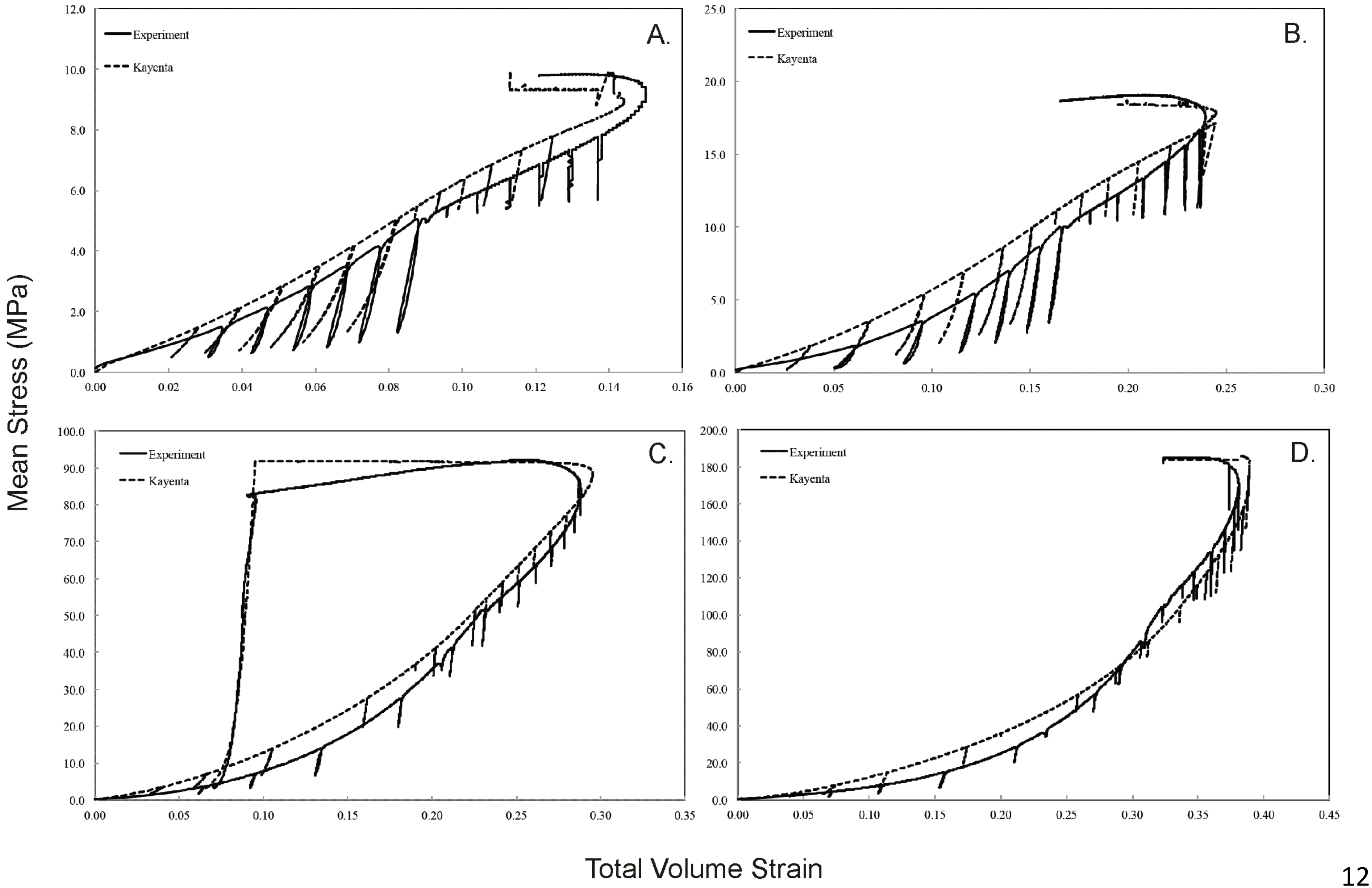
$$G = G_0\left(1 + G_1\sigma - G_2 \exp^{-G_3\sigma}\right)$$

- **NOTE:** bulk modulus was determined from the hydrostatic unloading portions

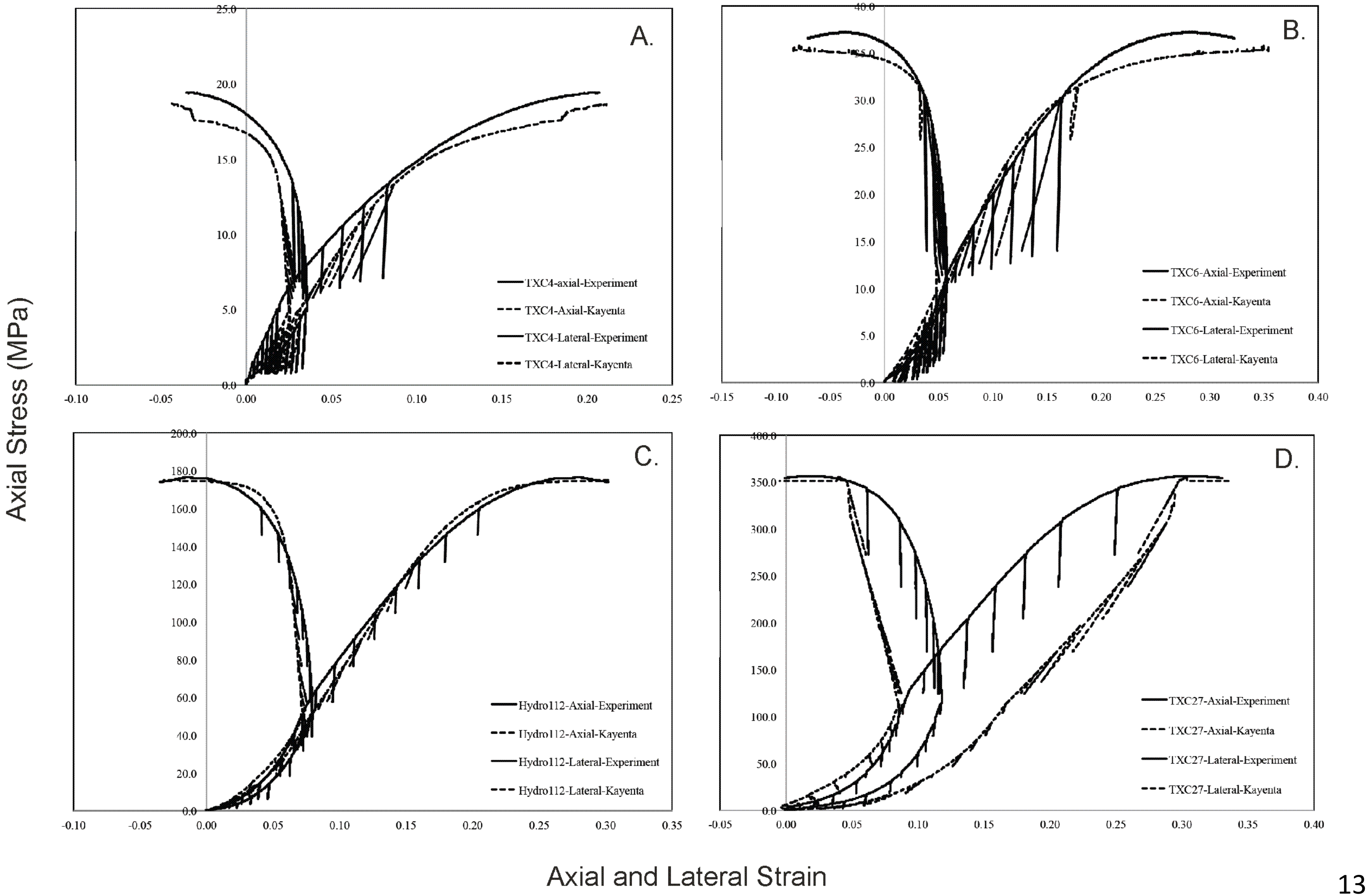
Kayenta constitutive modeling



Kayenta constitutive modeling



Kayenta constitutive modeling



Conclusion and recommendation

- Kayenta generates good descriptions of soil behavior over a broad range in mean and differential stresses.
- Tamped sample preparation results in anisotropic fabric.
- Crush curve formulations within Kayenta needs to be improved.

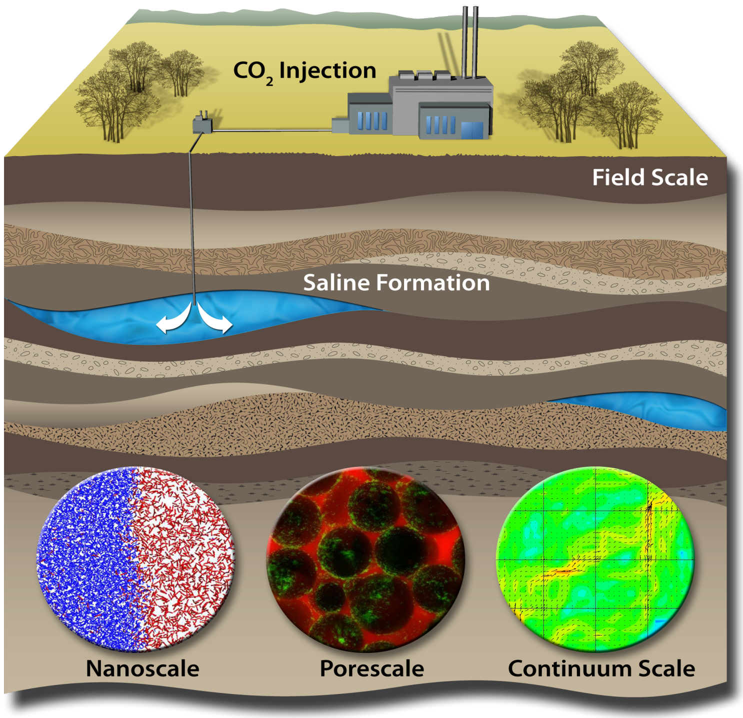
Select the right material model for your application purposes

Broome S.T., Flint G.M, Dewers T.A. and Newell P., Target soil impact verification: experimen- tal testing and Kayenta constitutive modeling, SAND report, SAND2015-9786, Sandia National Laboratories, 2014.

MULTI-SCALE, MULTI-PHYSICS COMPUTATIONAL MODELING OF SUBSURFACE

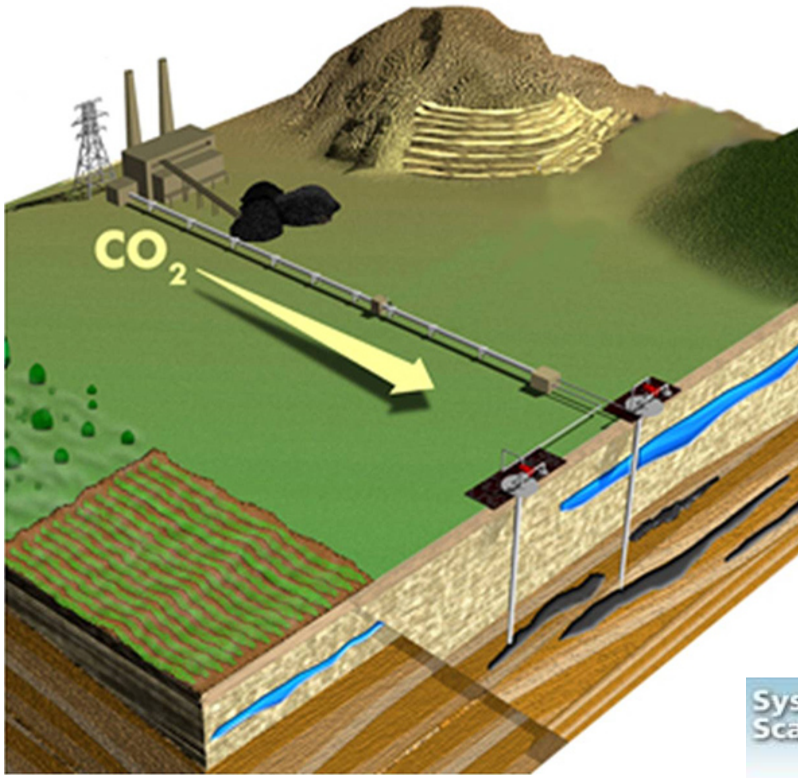
What is CO_2 sequestration?

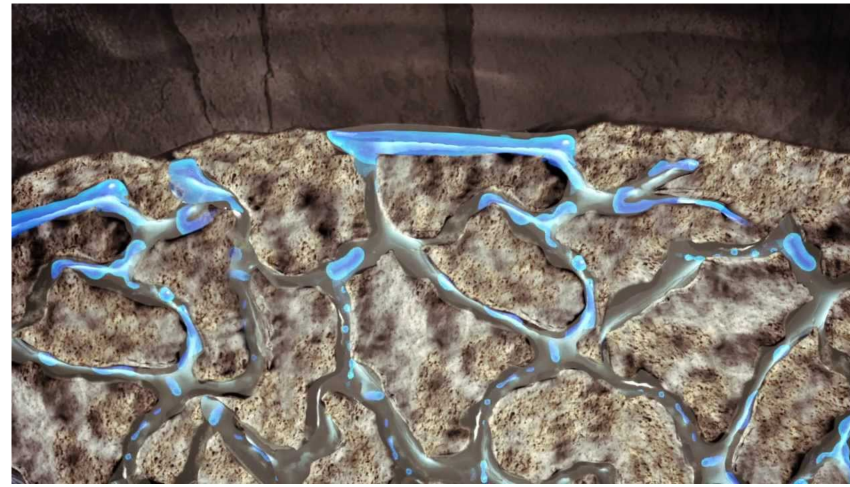
- **Carbon sequestration** is a potential tool to capture carbon from atmosphere or large scale sources such as power plants and store it into deep underground geological storage for long term.



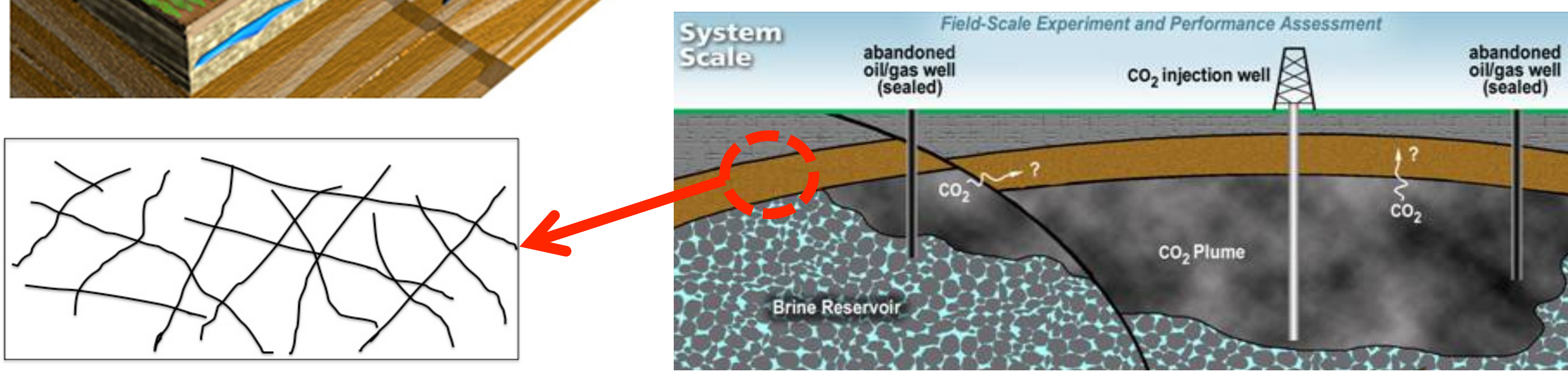
Courtesy: CFSES-SNL and UT-Austin

Safe and secure storage





Structural trapping-Youtube



Numerical model

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- Fluid:
  - Two phase, immiscible flow
  - The pore space is saturated
  - Capillary pressure is so small
  - No mass transfer between phases
- Mass balance equation:

ρ = Mass density
ϕ = Porosity
S = Saturation
k = Relative permeability
K = Intrinsic permeability tensor
p = Pore pressure
Q = Mass source
c = Capillary
w = wetting phase
n = non wetting phase

$$\frac{\delta(\rho_w \phi S_w)}{\delta t} = \nabla \cdot \left(\rho_w \frac{k_{rw}}{\mu_w} \underline{\mathrm{K}} \cdot (\nabla p_w - \rho_w \underline{\mathrm{g}}) \right) + Q_w$$

$$\frac{\delta(\rho_n \phi S_n)}{\delta t} = \nabla \cdot \left(\rho_n \frac{k_{rw}}{\mu_n} \underline{\mathrm{K}} \cdot (\nabla p_c + \nabla p_w - \rho_n \underline{\mathrm{g}}) \right) + Q_n$$

$$P_c = P_n - P_w$$

$$S_w + S_n = 1$$

Numerical model

- Solid:
  - Quasi static
  - Linear elastic
  - Balance of linear momentum:

$$\nabla . \sigma - \rho b = 0$$

$$\sigma = \lambda tr(\epsilon) I + 2\mu\epsilon$$

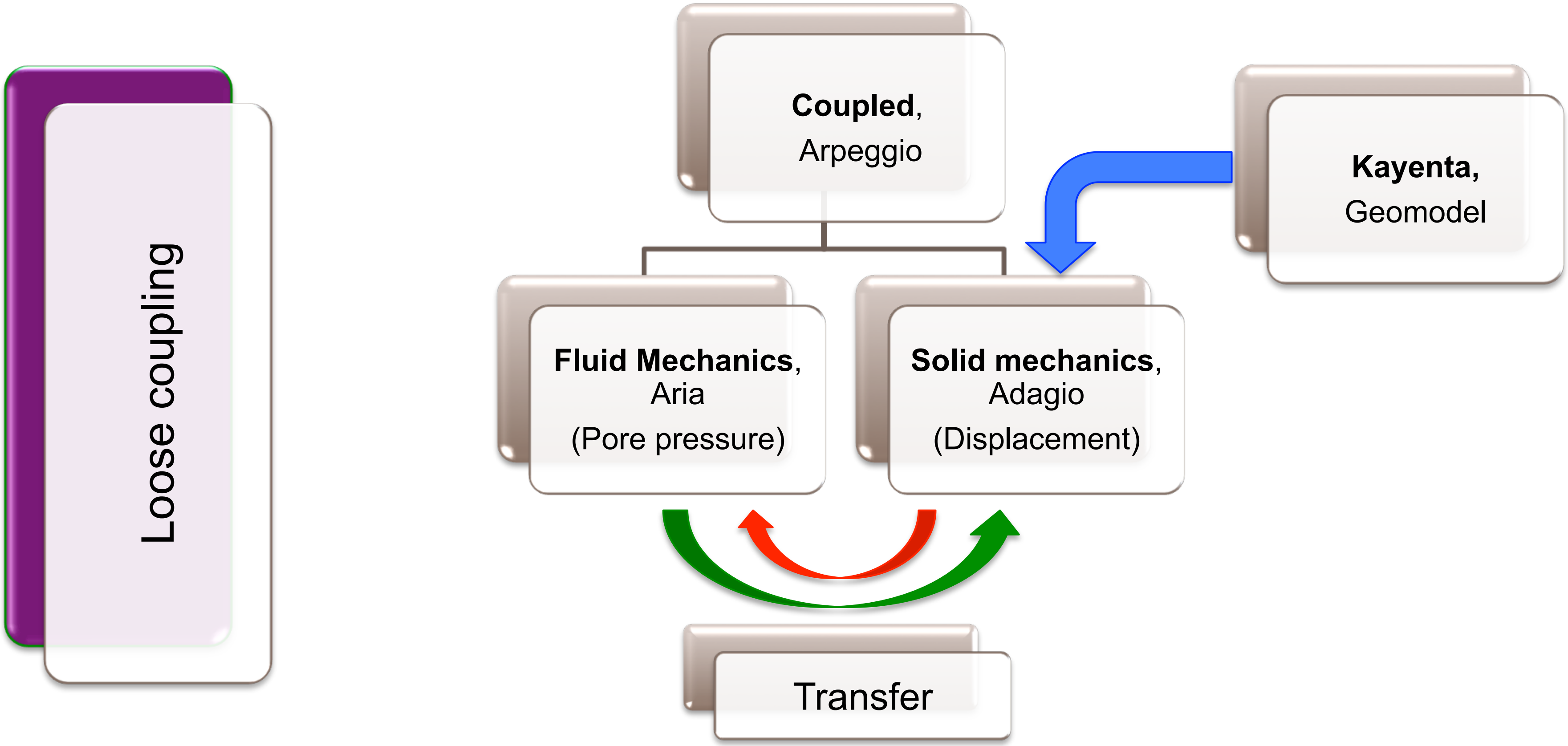
$$\epsilon = \frac{1}{2}[\nabla u + (\nabla u)^T]$$

- Coupling:

$$\sigma^{eff} = \sigma + \alpha I P$$

ρ = Mass density
b = Body force density
λ = Lame constant
σ = Cauchy stress tensor
ε = Strain tensor
μ = Shear modulus
u = Displacement field
α = Biot's coefficient
I = Identity tensor
P = Pore pressure

Sierra Mechanics



Aria: Galerkin FE program for coupled-physics problems described by systems of coupled PDEs
Adagio: 3-D, implicit, nonlinear Quasi-Statics; dynamics code
Arpeggio: Couples the Adagio, Aria, BEM, Calore and Premo Sierra Mechanics modules

Kayenta: quasi-static behavior of porous geomaterials

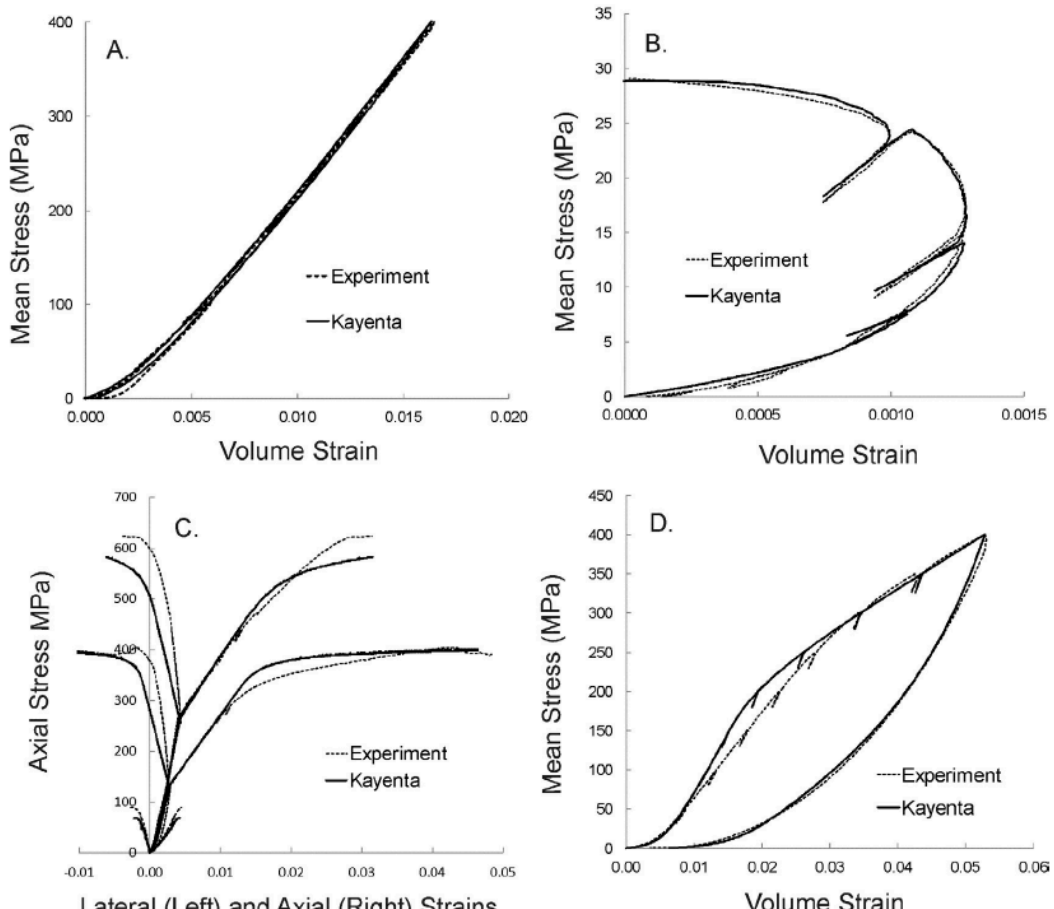
- Pressure sensitive
- Non-associative

plastic behavior

- Non-linear elasticity
- “Cap” yield surface

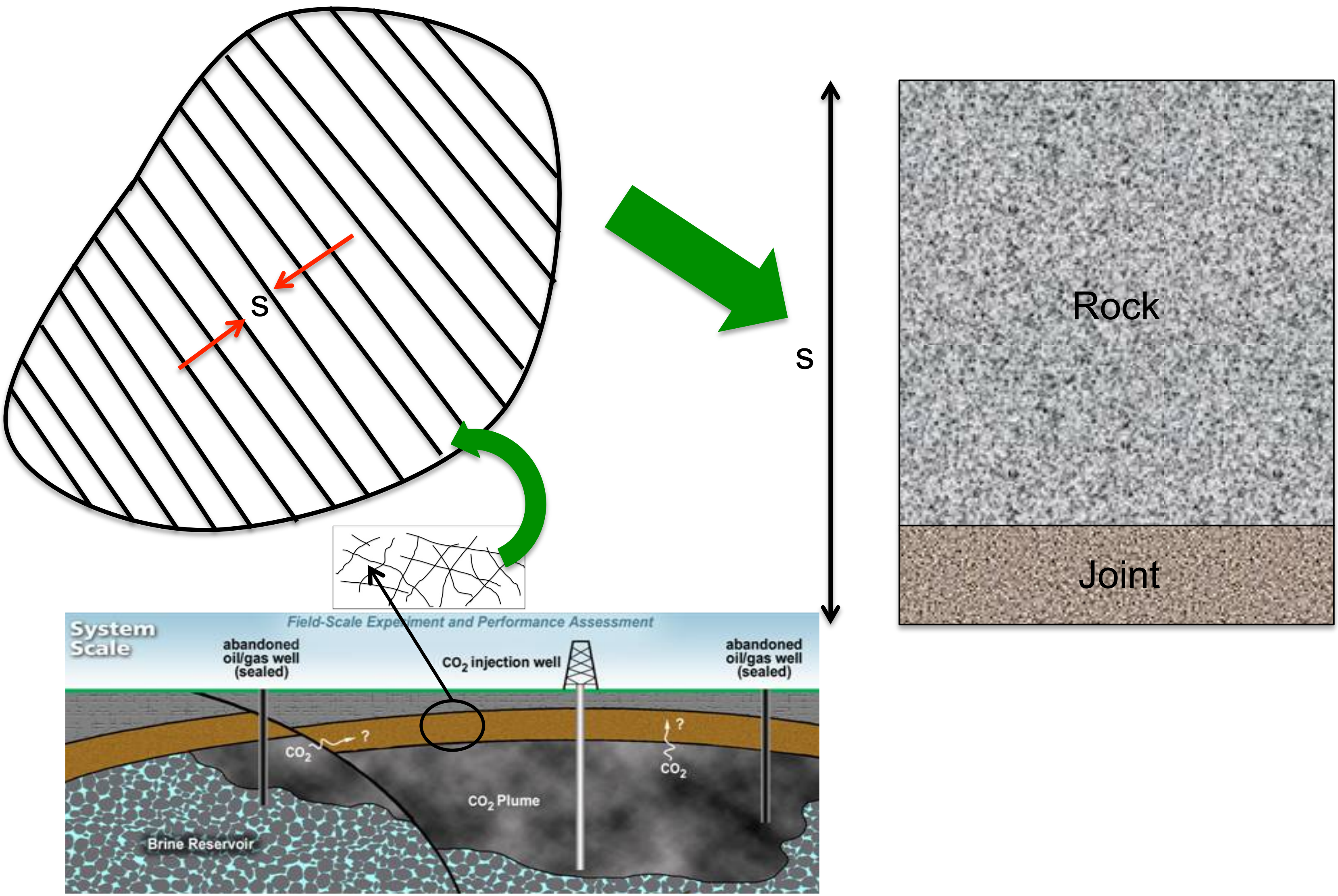
in stress space

- Shear-induced dilatation
- Note sign conventions!!!



Dewers T. A., Newell P., Broome S., Heath J. and Bauer S., Geomechanical behavior of Cambrian Mount Simon Sandstone reservoir lithofacies, Iowa Shelf, USA, *International Journal of Greenhouse Gas Control*, 2013, Vol. 21, February 2014, pp 33-48.

Equivalent continuum model-Kayenta



Formulation

Coupling

$$K_{eff} = K_R + \sum_{J=1}^{n} K_J$$

$$n_1 = \sin\alpha \sin\beta$$

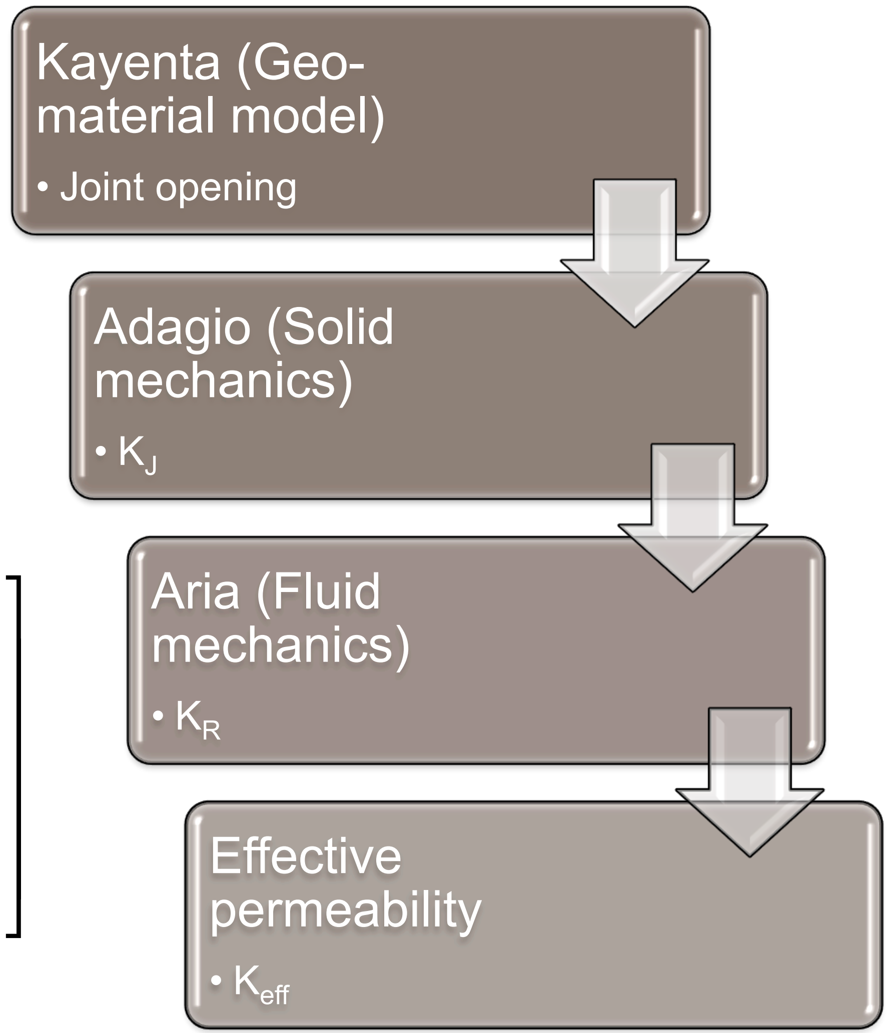
$$n_2 = \sin\alpha \cos\beta$$

$$n_3 = \cos\alpha$$

Joint opening

$$K_J = \frac{b^3}{12s}\begin{bmatrix} 1-n_1^2 & -n_1 n_2 & -n_1 n_3 \\ -n_1 n_2 & 1-n_2^2 & -n_2 n_3 \\ -n_1 n_3 & -n_2 n_3 & 1-n_3^2 \end{bmatrix}$$

Joint spacing



Formulation

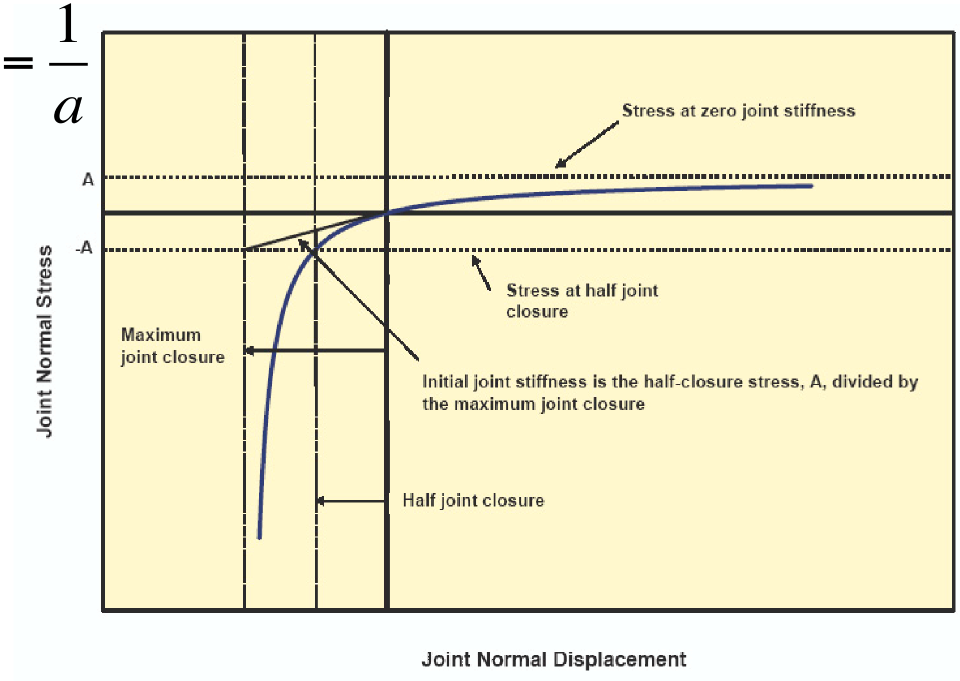
$$\sigma = \frac{\varepsilon}{A + B\varepsilon} \Rightarrow \sigma_n = \frac{U_n}{a + bU_n}$$

$$when\ \ \sigma_n \to \infty \Rightarrow U_n \to \frac{-a}{b} = V_{\max}$$

$$when\ \ \sigma_n \to 0 \Rightarrow U_n \to 0 \Rightarrow k_{ni} = \frac{1}{a}$$

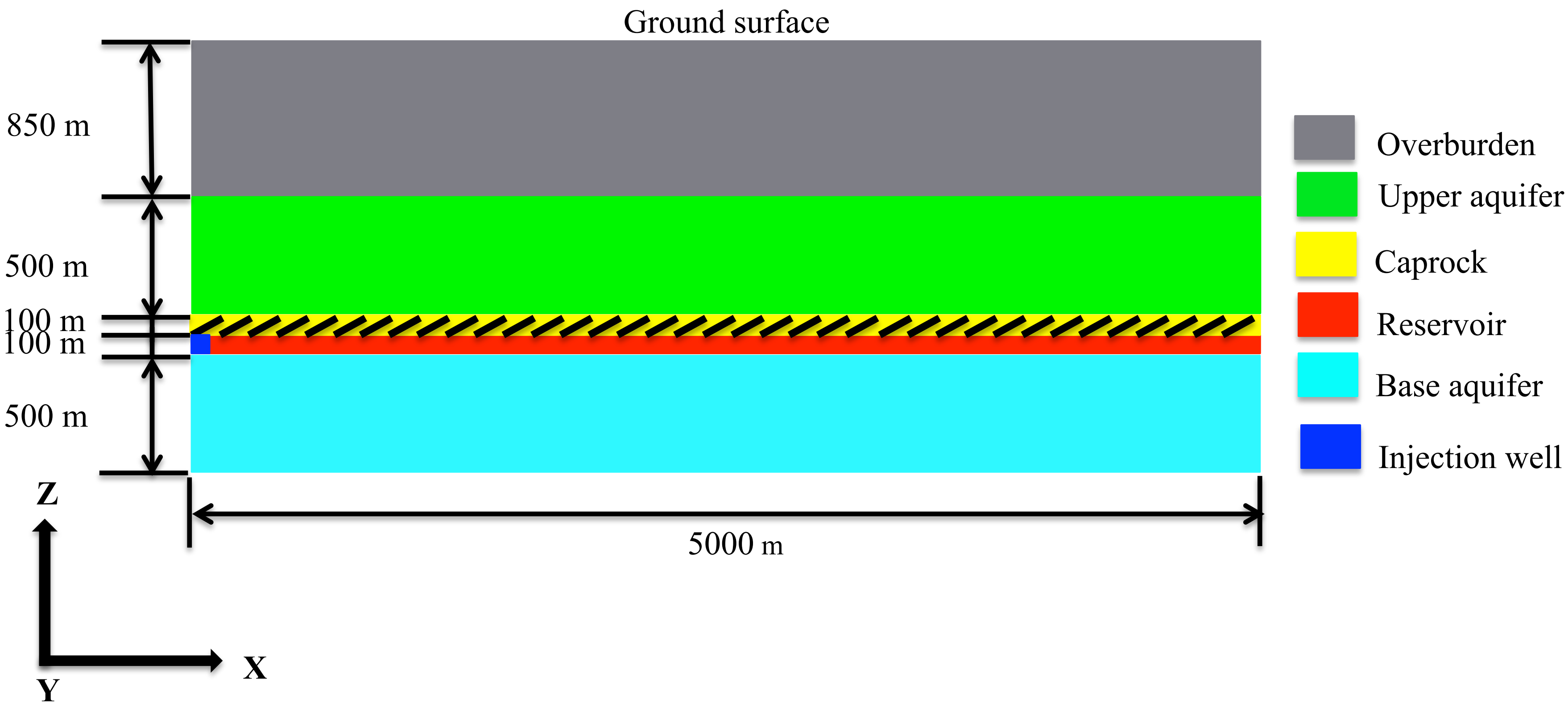
$$b = \frac{V_m}{1 - \frac{\sigma_n}{k_{ni}V_m}} - \frac{V_m}{1 - \frac{\sigma_{ni}}{k_{ni}V_m}}$$

$$k_n = \frac{\partial \sigma_n}{\partial U_n} \Rightarrow k_n = k_{ni}\left(1 - \frac{\sigma_n}{k_{ni}V_m}\right)^2$$



Brannon et al., 2009

Schematic of the jointed caprock



Properties

- Solid

Property	Aquifer	Caprock	Injection zone	Base	Units
Density	2100	2100	2100	2100	Kg/m^3
Biot's coefficient	1	1	1	1	
Young's modulus	20	50	20	50	GPa
Poisson's ratio	0.2	0.12	0.2	0.12	

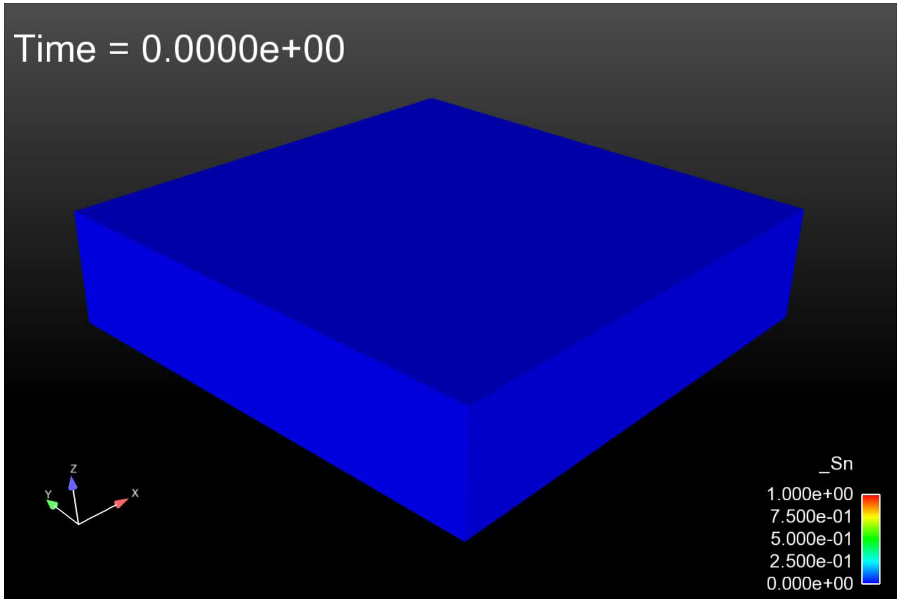
- Fluid

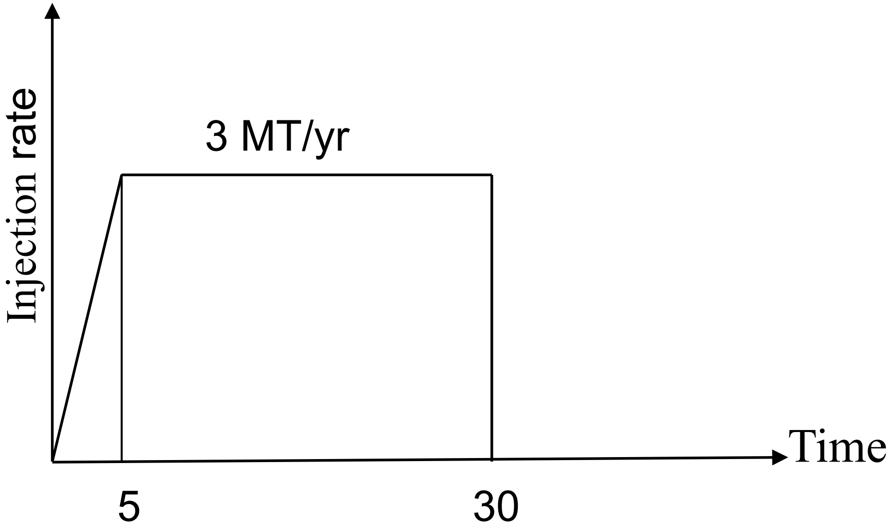
Property	Aquifer	Caprock	Injection zone	Base	Units
Initial porosity	0.15	0.05	0.15	0.10	
Intrinsic permeability	$2x10^{-14}$	$1x10^{-18}$	$2x10^{-14}$	$1x10^{-16}$	m^2

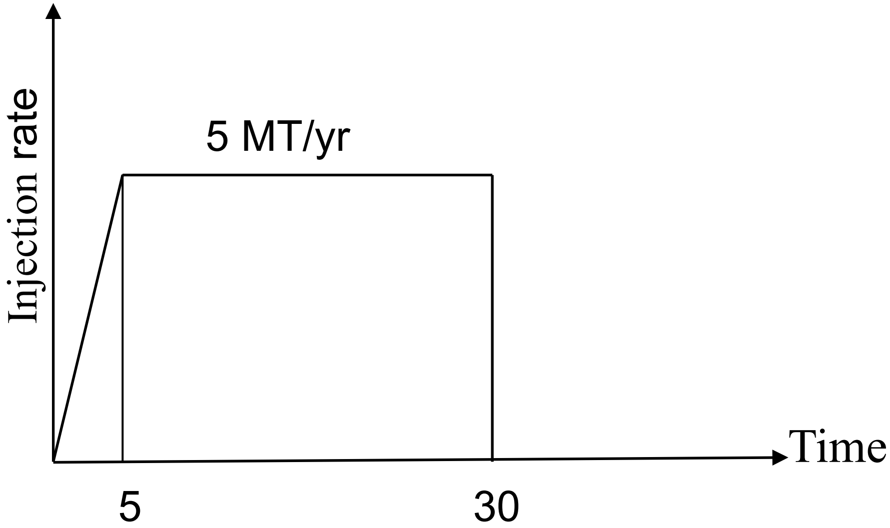
- Joint

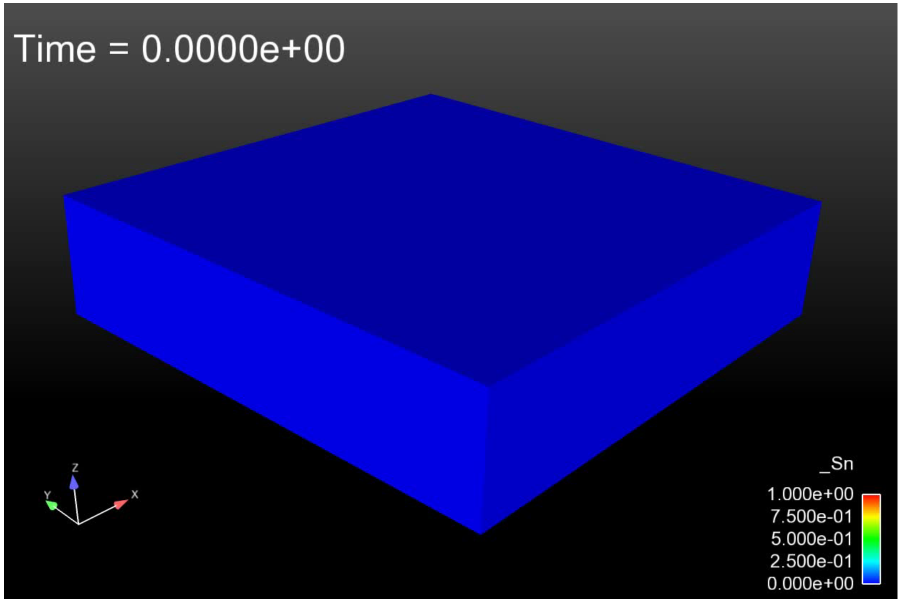
Joint		
K_{ni} (Pa)	V_{max} (m)	S (m)
$1.5x10^{+10}$	$7.5x10^{-5}$	1.00

Injection rate impact

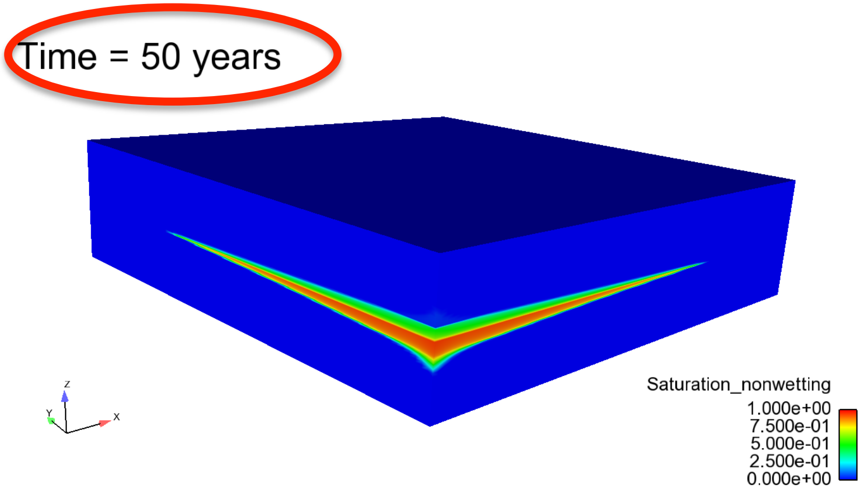




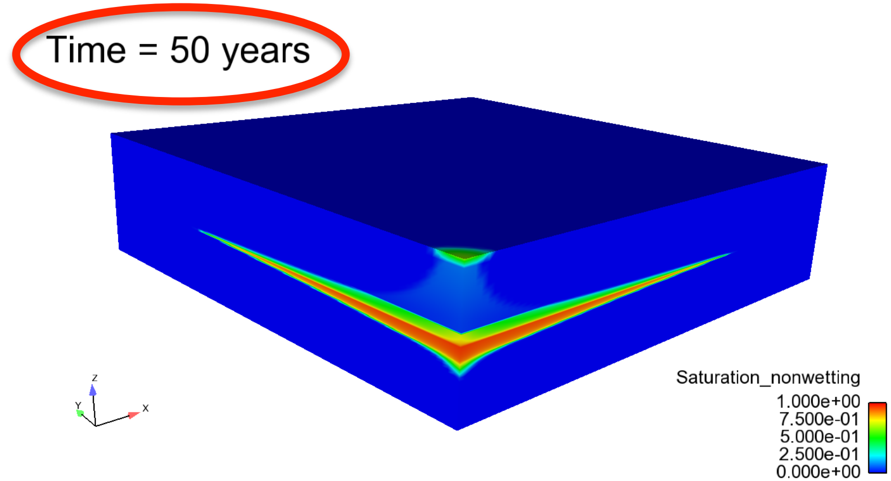




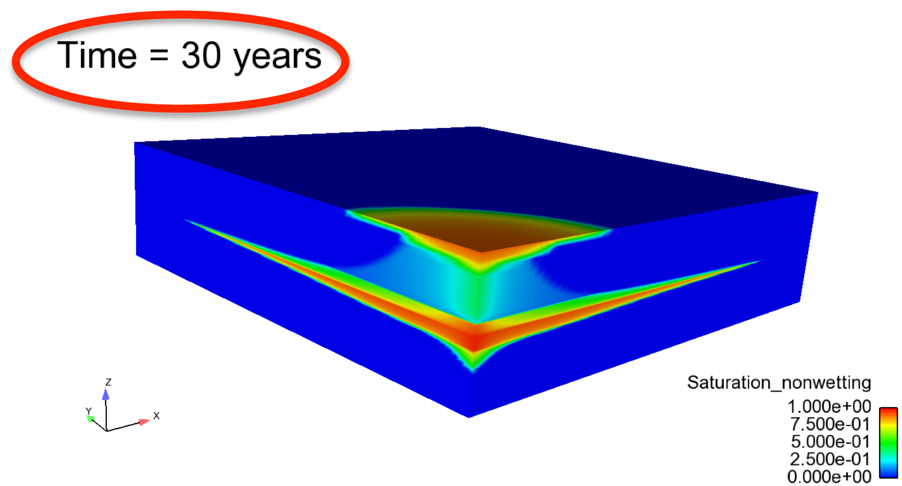
Results



The saturation of nonwetting phase for case without joint- 3Mt/yr, after 50 years of injection.



The saturation of nonwetting phase for case with joint-3 Mt/yr, after 50 years of injection.



The saturation of nonwetting phase for case with joint-5 Mt/yr, after 30 years of injection.

Conclusions

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- It is critical to include preexisting joints/fractures in caprock integrity analysis.
- Effective permeability within the caprock increases by increasing the injection rate.
- The leakage increases by increasing the injection rate.

Capturing the physics of the problem with right material model and computational tools

Martinez M.J., **Newell P.**, Bishop J.E. and Turner D.Z., Coupled multiphase flow and geomechanics model for analysis of joint reactivation during CO2 sequestration operations, International Journal of Greenhouse Gas Control, Vol. 17, September 2013, pp. 148-160.

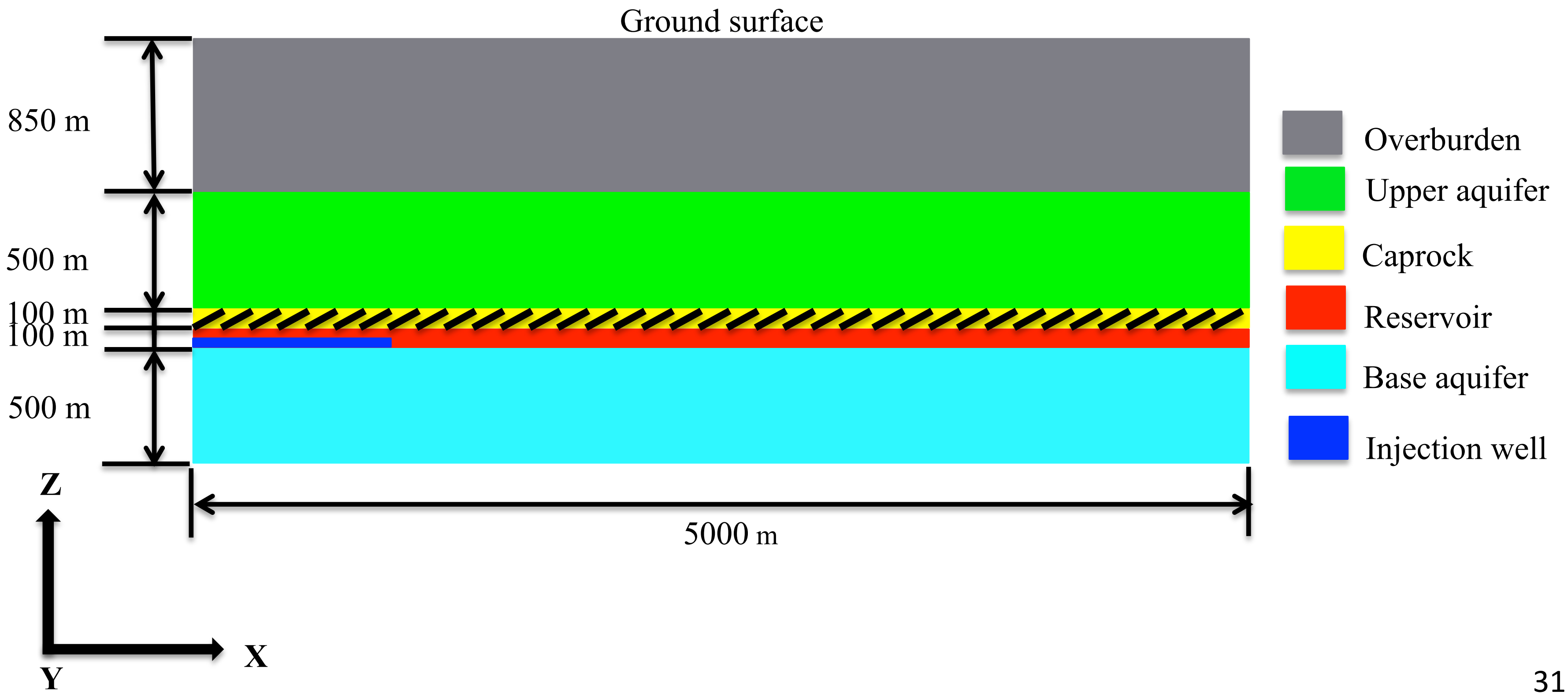
Martinez M.J., **Newell P.**, and Bishop J.E., Coupled multiphase flow and geomechanics for analysis of caprock damage during CO2 sequestration operations, Proceedings. XIX International Conference on Water Resources CMWR 2012, Univ. of Illinois, Champaign IL., June 17-22, 2012.

Additional slides

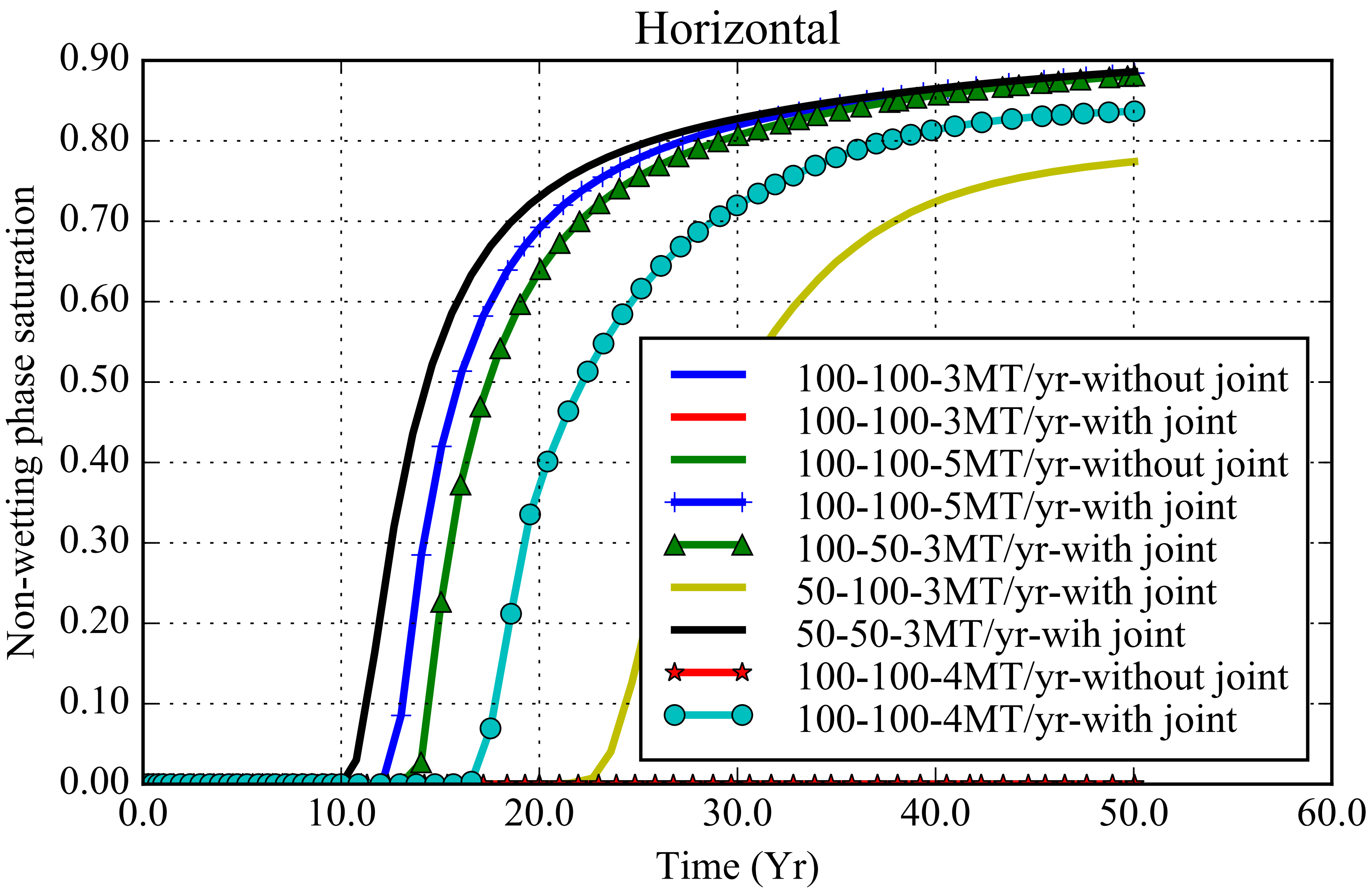
- If time permits

Horizontal wellbore

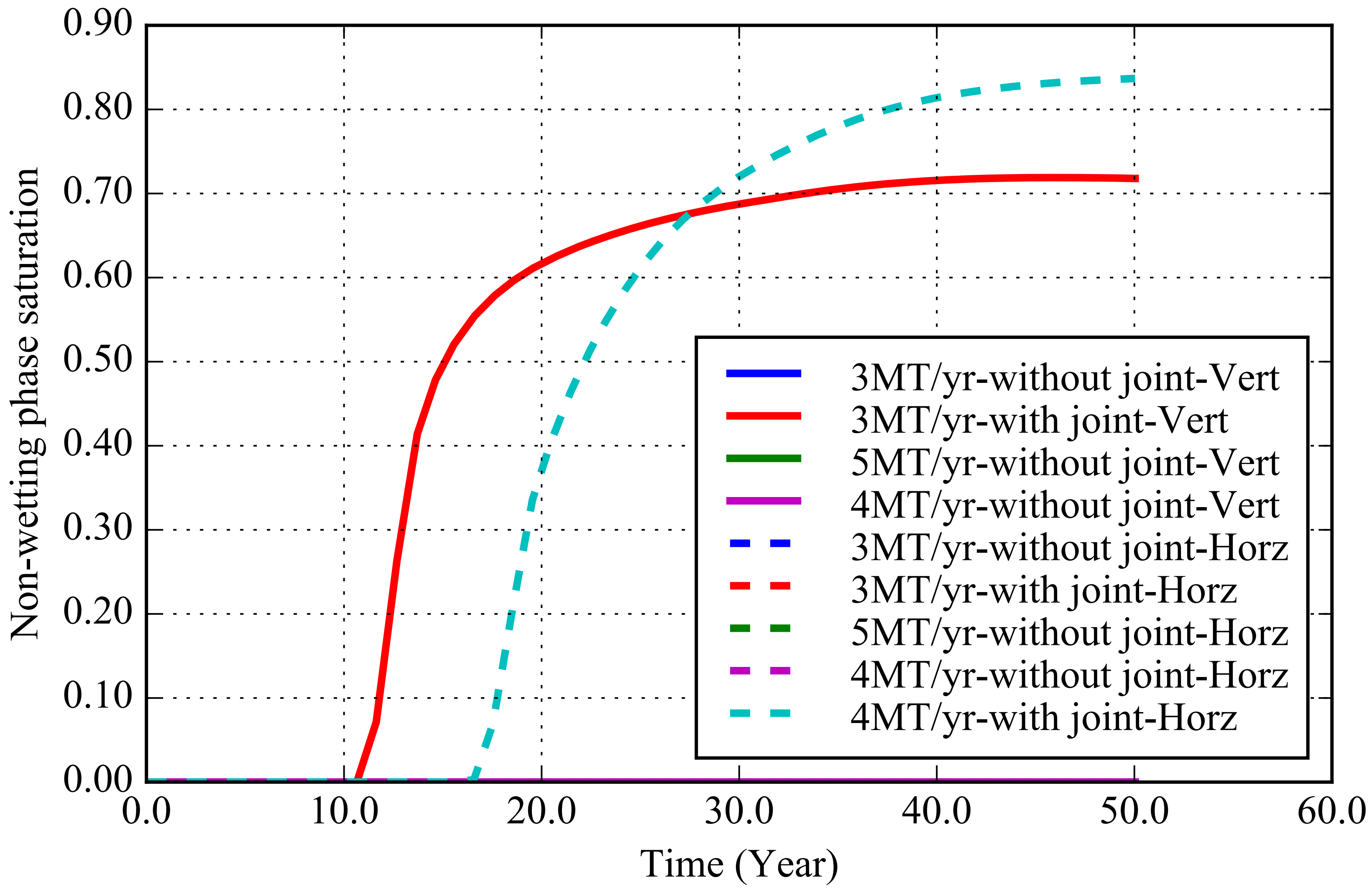
	Case	Reservoir thickness (m)	Caprock thickness (m)	Joint orientation (Degree)
Base case	1	100	100	No joint
Geometric	2	100	100	90
	3	100	50	90
	4	50	100	90
	5	50	50	90



Horizontal wellbore



Wellbore orientation



Wellbore orientation