Coupled HCTM Phenomena

From Pore-scale Processes to Macroscale Implications

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U.S. Department of Energy

National Energy Technology Laboratory
Carbon Storage R&D Project Review Meeting
Developing the Technologies and Building the
Infrastructure for CO_2 Storage

August 21-23, 2012

Presentation Outline

Project Overview:	*The Proposal*
Accomplishments:	HTCM Coupled Processes
Appendices:	Contact Information
	Schedule
	Bibliography

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Relevance

"Faustian bargain"?

long-term CO_2 geo-storage needed (C-economy + climate change)
but, it must be reliable in the long time scales

High early probability of failure

new engineering solutions: high initial P_f (emergence phenomena)

Main concerns

complex geo-plumbing

unanticipated coupled hydro-chemo-thermo-mechanical processes

unrecognized emergent phenomena (including positive feedbacks)

Without paralyzing critically needed CCS, make all efforts to

anticipate potential challenges
develop proper engineering solutions

This has been the purpose of this research

Project Objectives / Goals

better understanding of fundamental processes and couplings that may either hinder or enhance the long-term C-geological storage

To reach this goal, we will:

- explore the geomechanical consequences of *HCTM on* geo-storage of CO_2
- identify emergent phenomena
- bound the parameter-domain for efficient injection and safe long-term storage

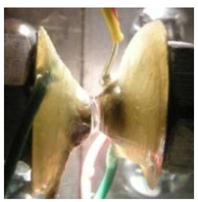
Approach combines:

- fundamental pore and particle-scale experimental studies
- upscaling numerical simulations
- macroscale numerical modeling

1D | 2D | 3D - σ’

1D

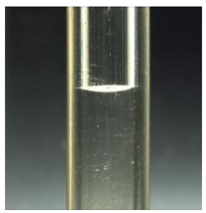
Contact



grain-grain

dissolution

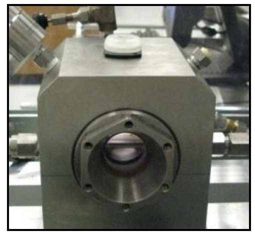
Short Capillary

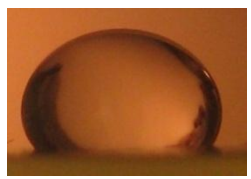


Interface

diffusion

Droplet



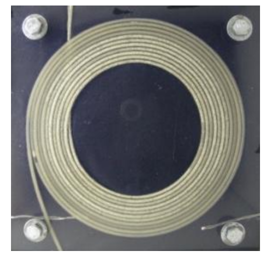


surface tension

contact angle

solubility

Long Capillary



mixed fluid

2D

2D Cell

2D observations

2D invasion

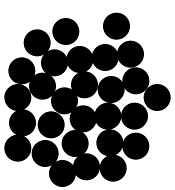
transients

3D - σ’

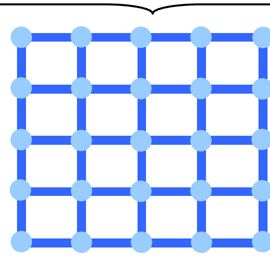
Sediment

sediment

fracture



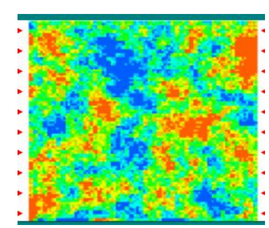
DEM - PFC



Network Model

$$\frac{\partial}{\partial t}\left[\rho_g S_g\right]\phi + \nabla.\left[\rho_g \mathbf{q}_g\right] \sim f^m$$

Analytical

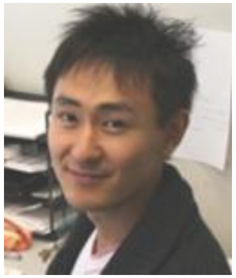


FEM: Code-bright

Project Team

N Espinoza (ENPC)

θ T_s CO_2-CH_4 Clays



SH Kim

HC coupling - NM

A. Sivaran

leaks - cements

H.S. Shin (Ulsan U)

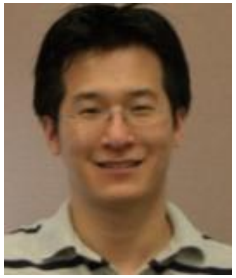
Dissolution DEM

ES Bang (KIGAM)

Monitoring

J.W. Jung (LSU)

CO_2-CH_4



J. Jang (WSU)

Network Models

M.S. Cha

Dissolution - DEM

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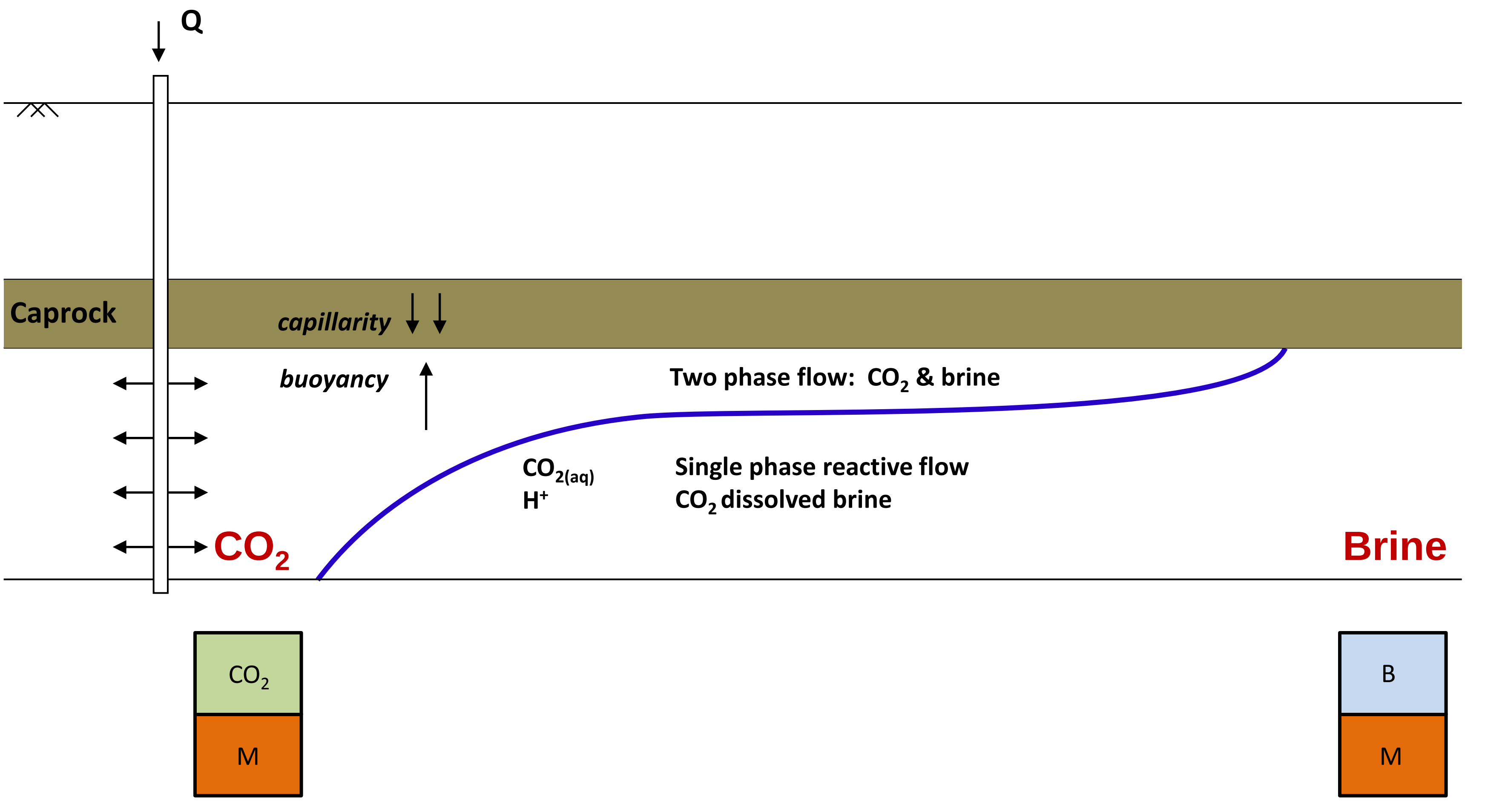
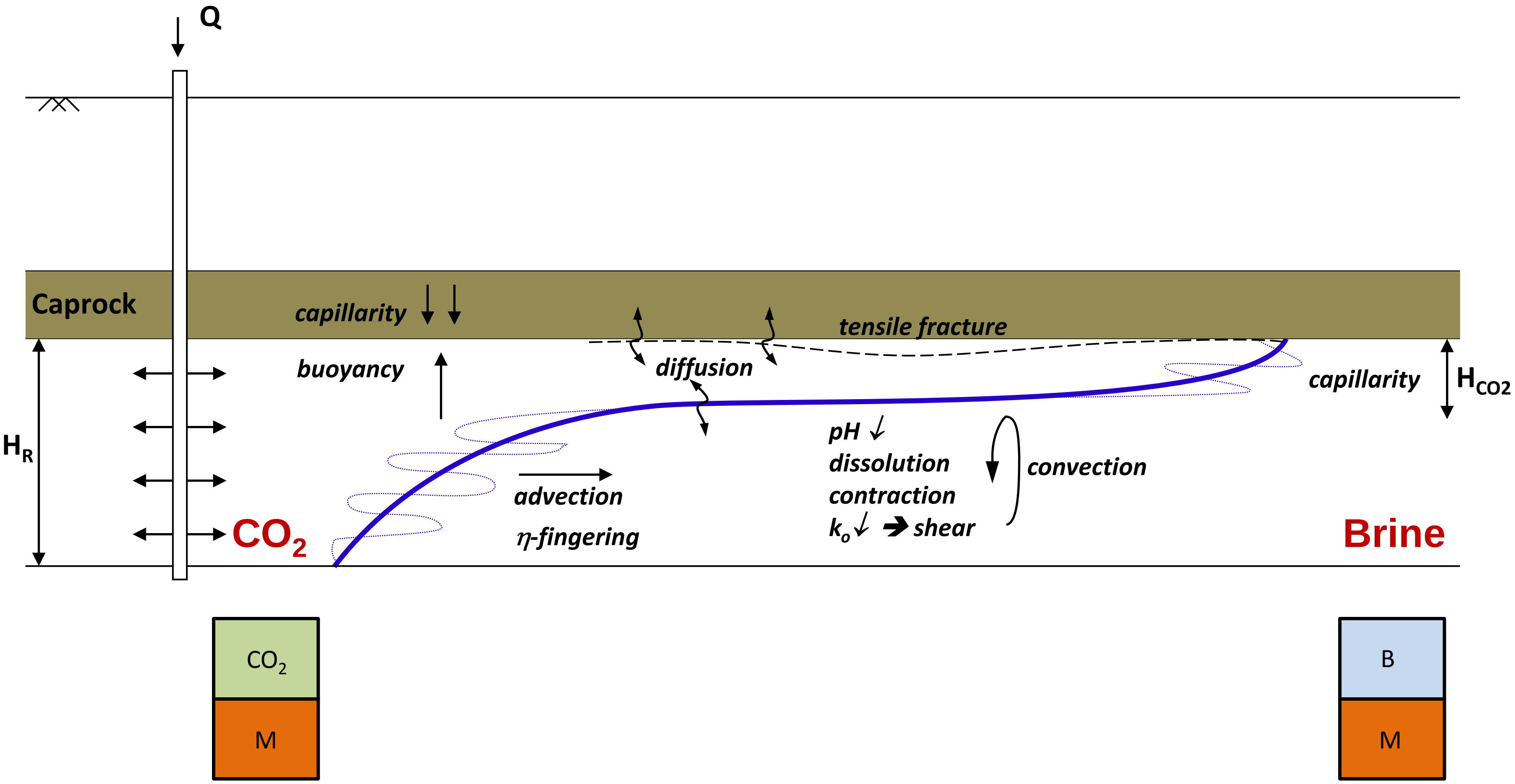
preliminary analyses

Reservoir - Zones



Reservoir - Zones



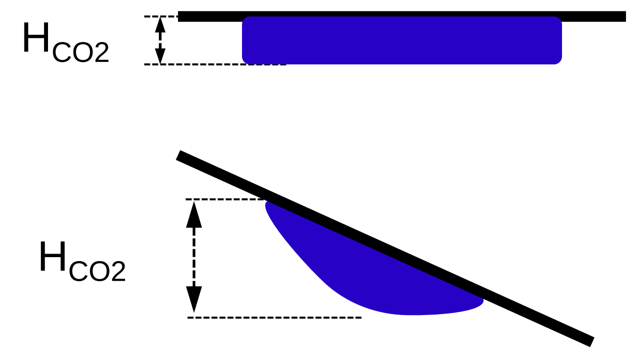
CO_2 plume thickness (without a trap)

$$p_{CO2} - p_w = H_{CO2}(\gamma_w - \gamma_{CO2})$$

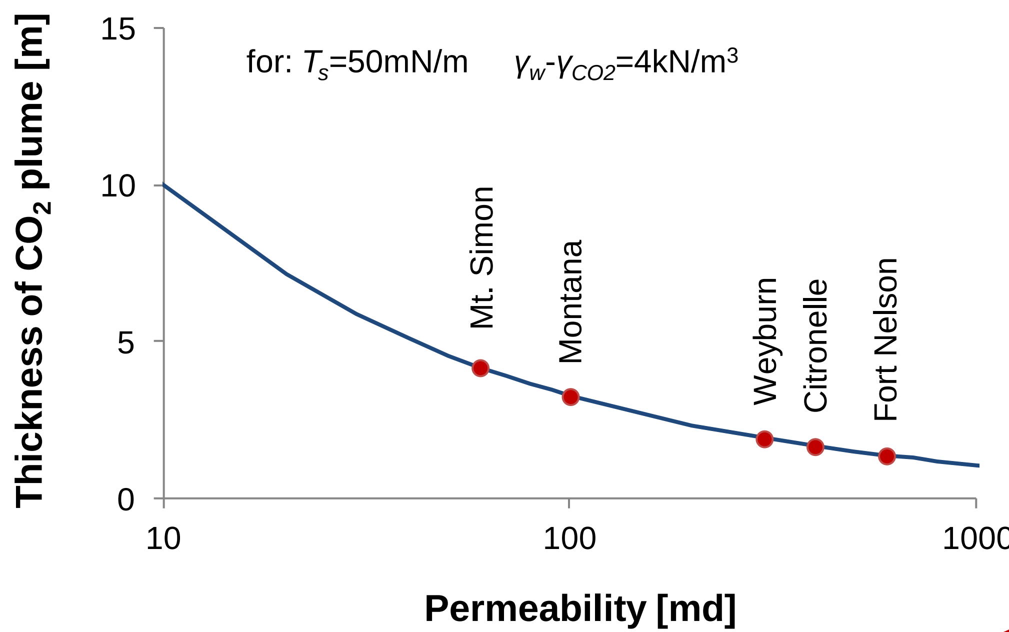
$$p_{CO2} - p_w = \frac{2T_s}{R_{pore}}$$

$$\frac{k_{perm}}{md} \approx 2\left(\frac{R_{pore}}{\mu m}\right)^2$$

after Bachu and Bennion (2008)



$$H_{CO2} = \frac{2T_s}{R_{pore}(\gamma_w - \gamma_{CO2})}$$

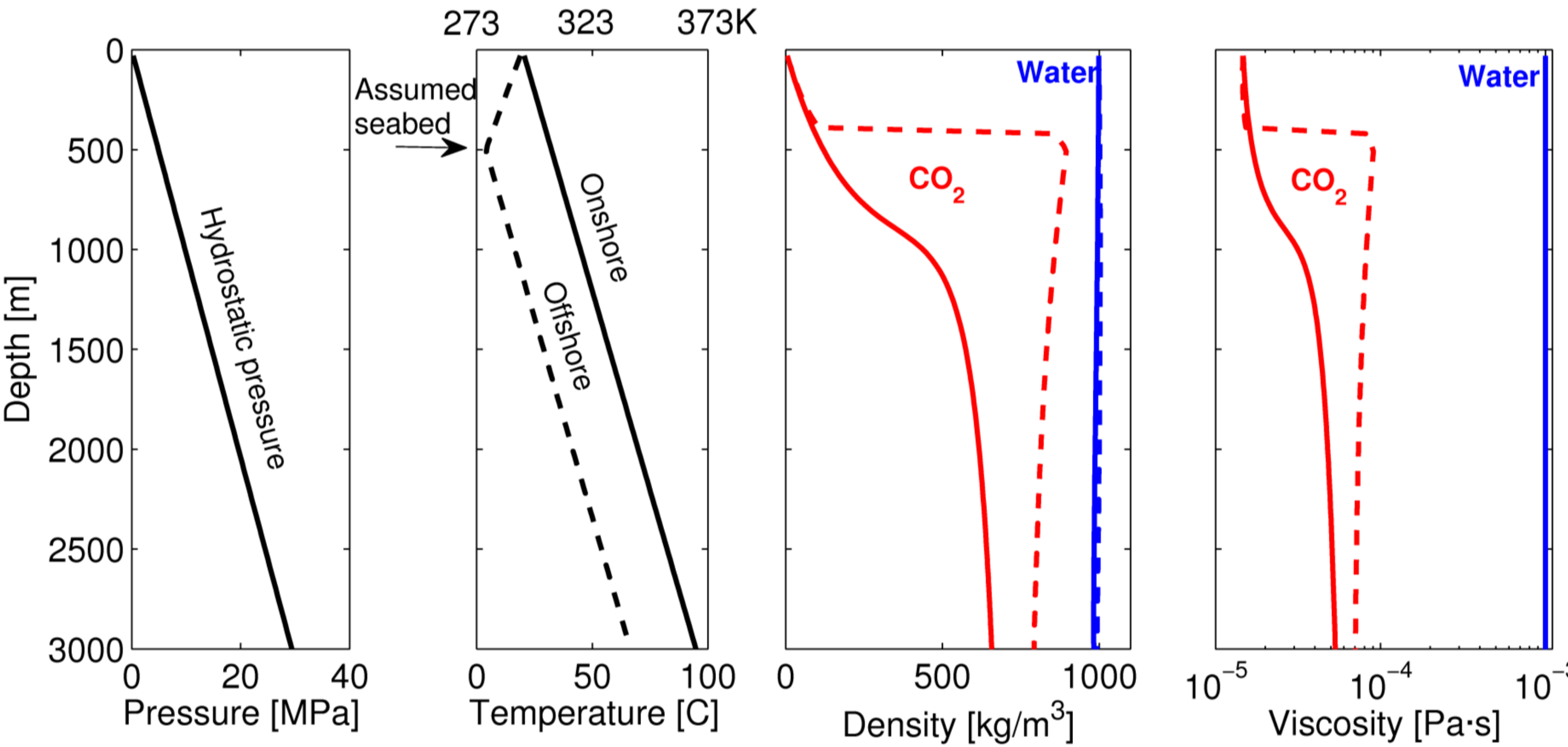


water + CO_2

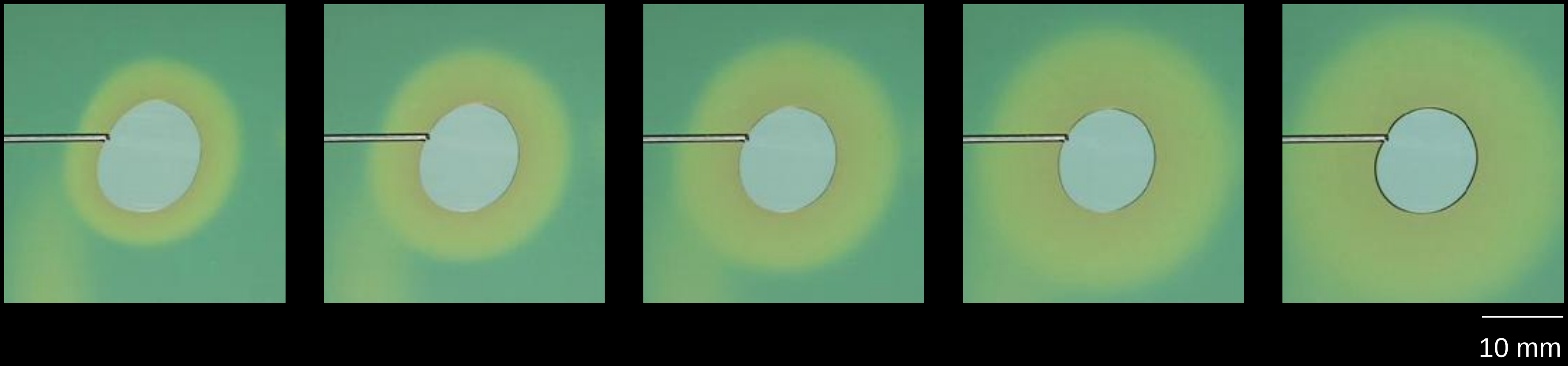
Physical Properties

Property	CO_2 liquid	H_2O liquid
Mechanical		
Viscosity μ [Pa·s]	(2-to-8)×10^{-5} [5-to-30MPa, 318K]	~1.5×10^{-3} [293K]
Density *ρ* [kg·m^{-3}]	~938-to-800 kg/m^3 [10MPa, 280-to-300K] (highly variable)	999.9 [0.1MPa, 273K] 1003±1.5 [10MPa, 280-to-300K]
Coefficient of thermal expansion *α* [K^{-1}]	No data found	2±0.3×10^{-4} [50MPa, 273.15-to-283.15K]
Bulk Modulus [GPa]	0.338-to-0.124 GPa [10MPa, 280-to-300K]	2.1-to-2.3 GPa [10MPa , 280-to-300K]
Shear Modulus [GPa]	0	0
Poisson ratio	~0.5	~0.5
V_P [m/s]	~600-to-400 m/s [10MPa ,280-to-300K]	1450-to-1518 [10MPa ,280-to-300K]
V_S [m/s]	0	0

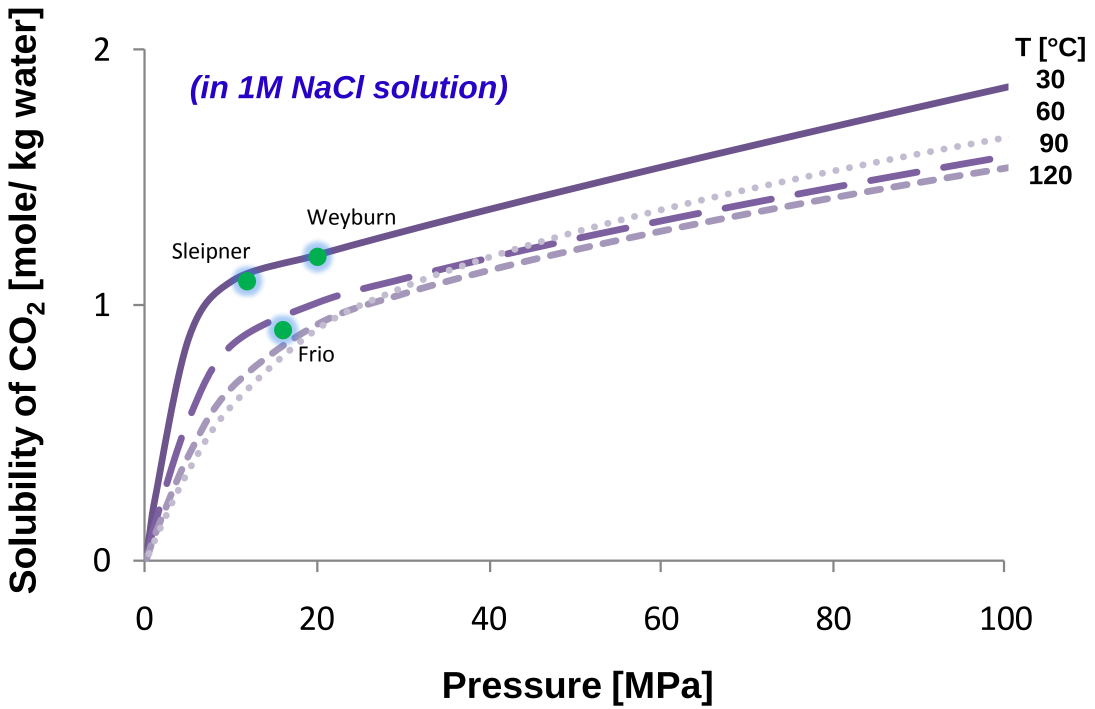
Physical Properties: Onshore vs Offshore



CO_2 Dissolution and H_2O Acidification

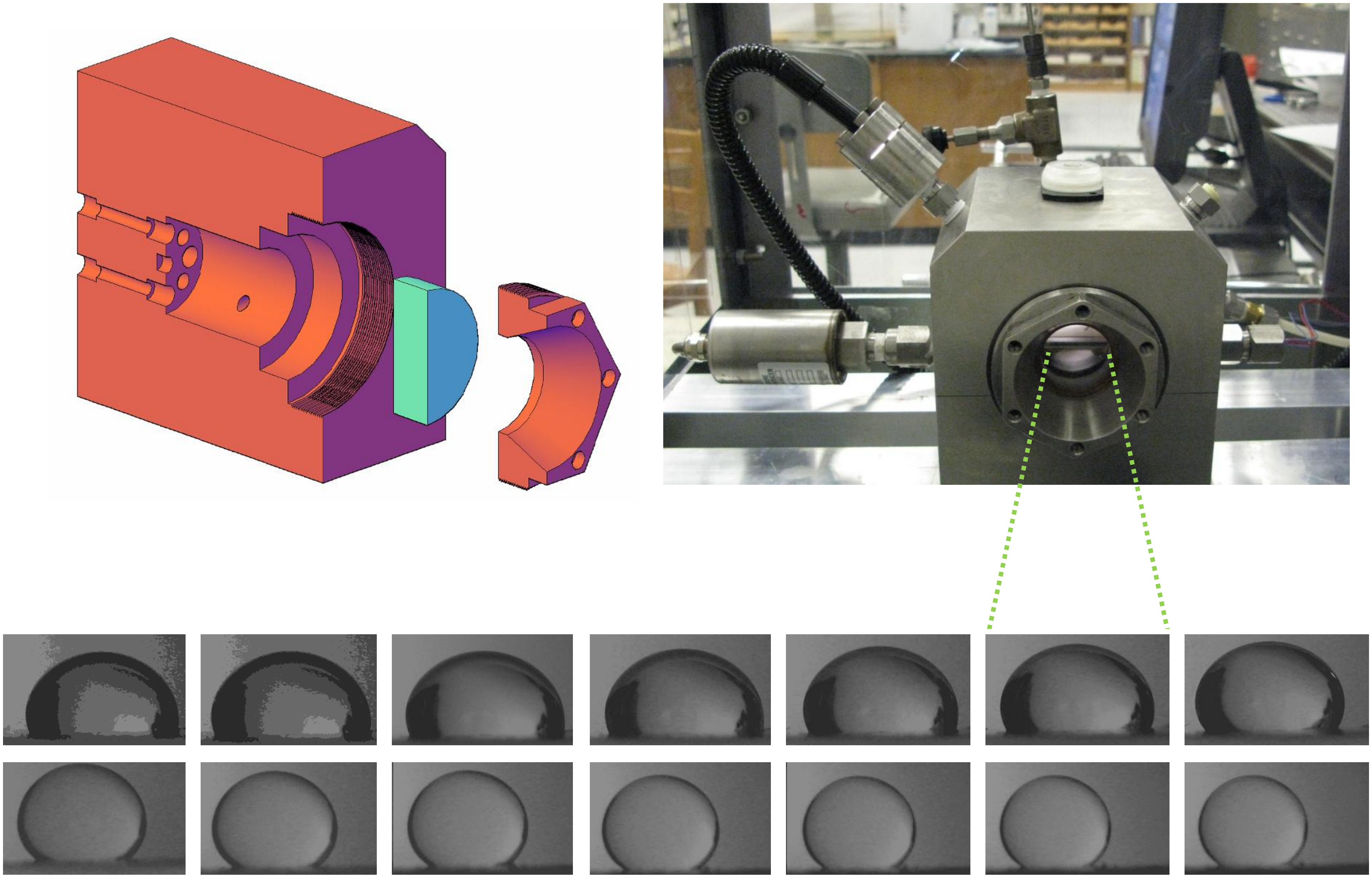


CO_2 Solubility in Water

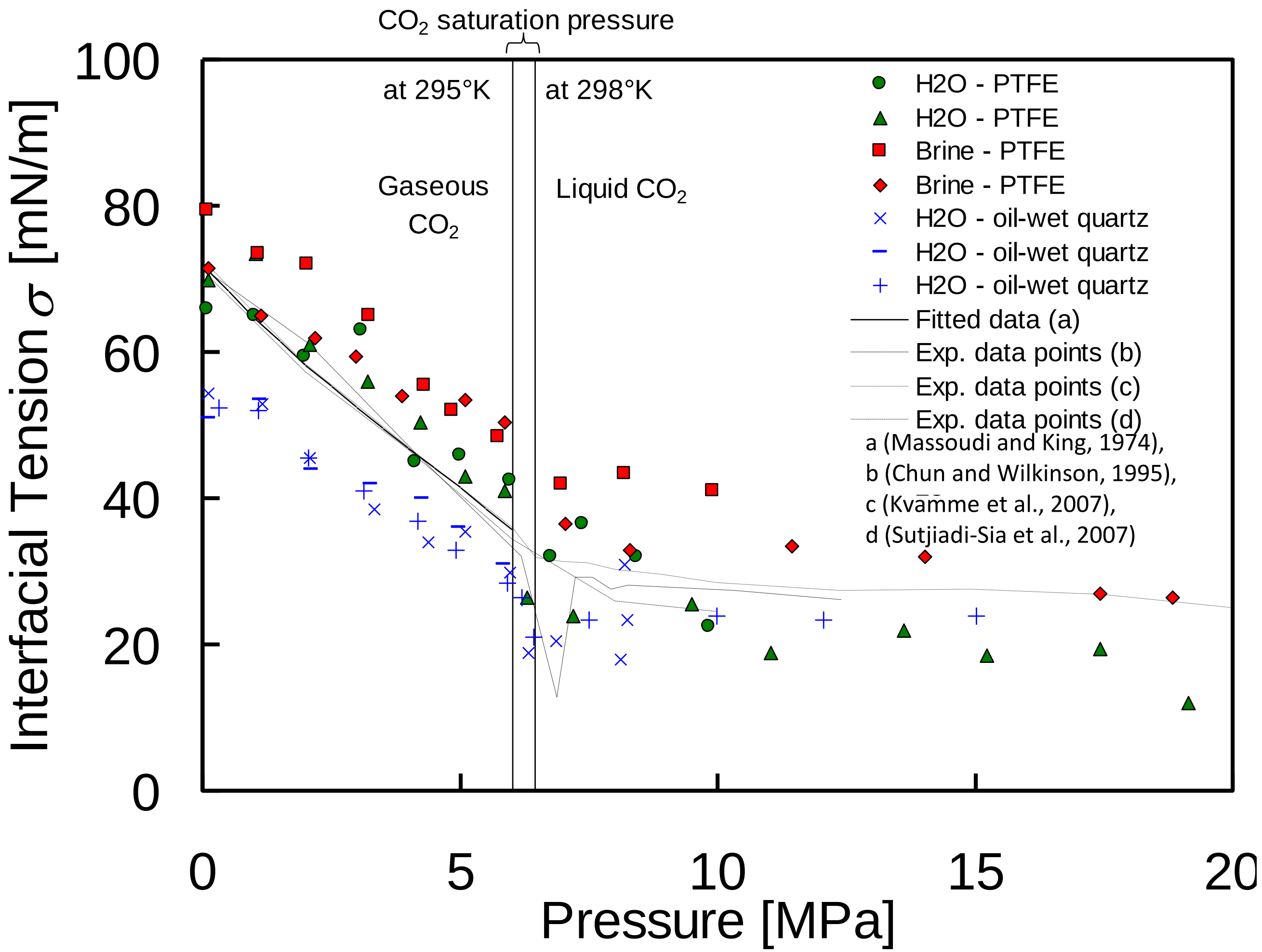


Duan and Sun (2003)

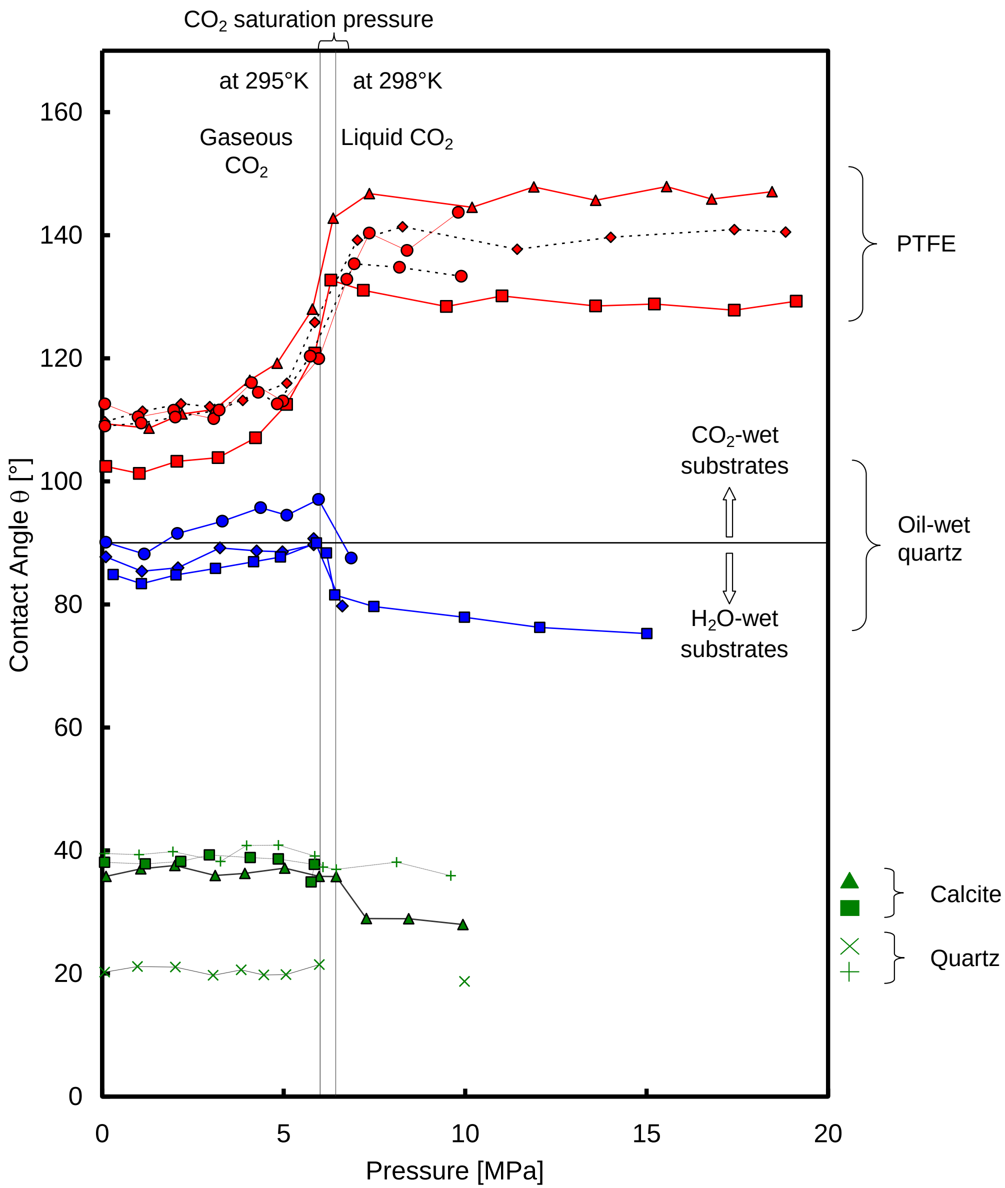
Surface Tension and Contact Angle

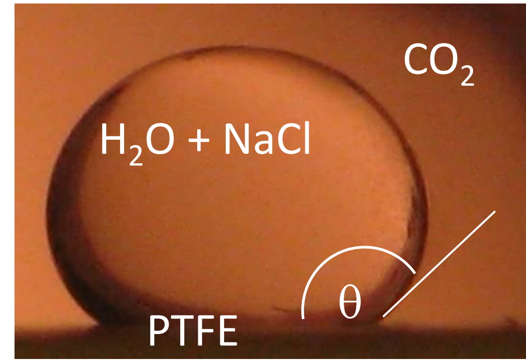


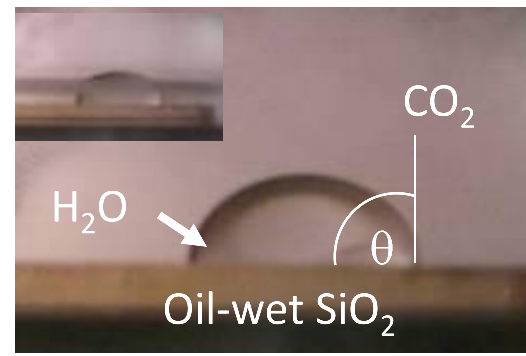
Surface Tension

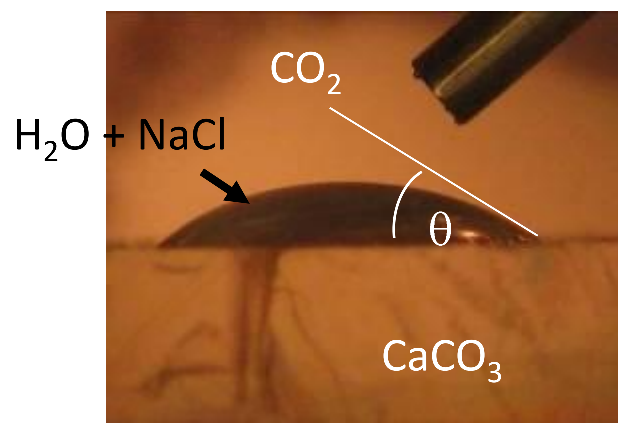


Contact Angle

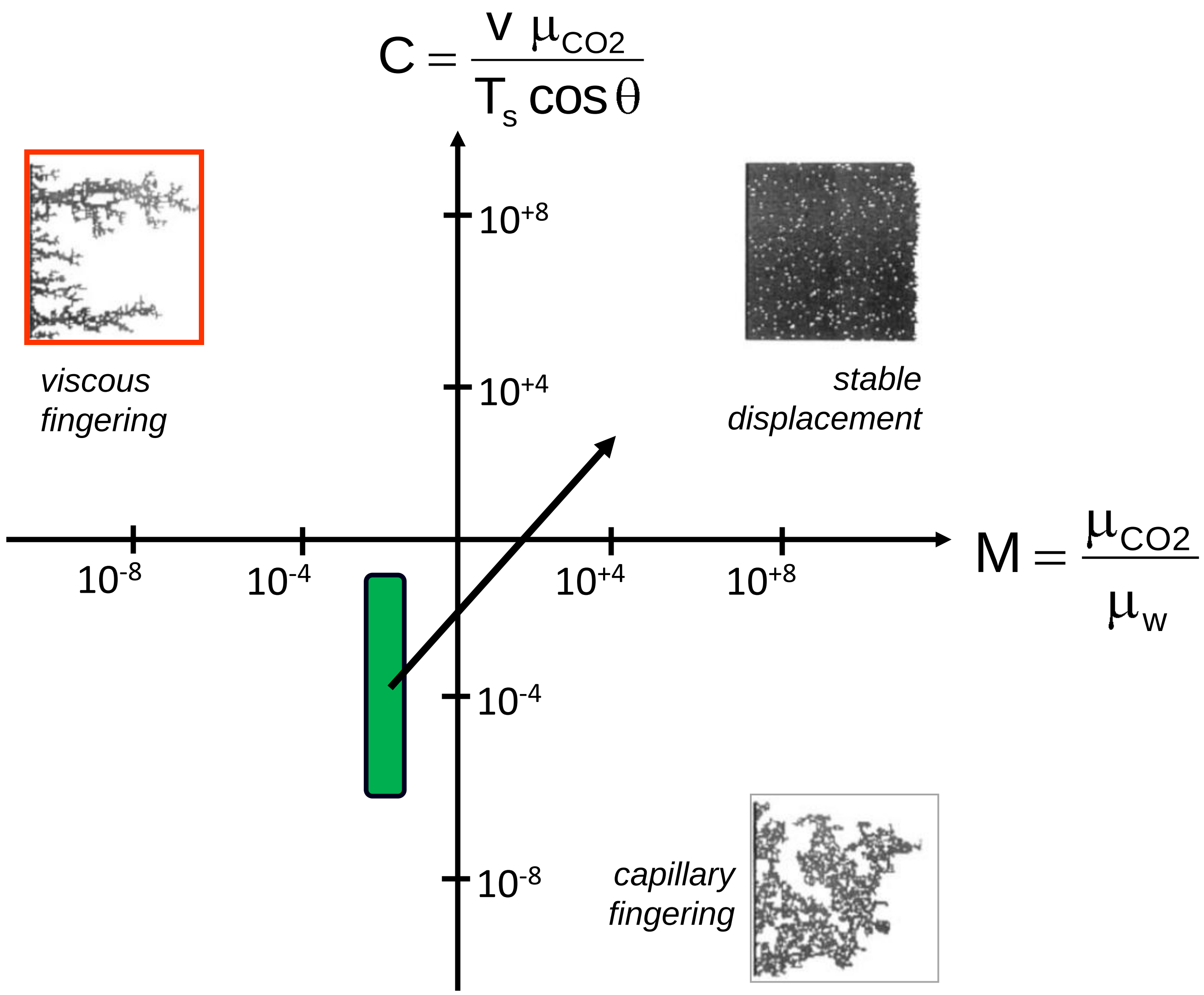








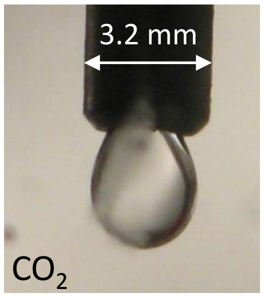
Invasion = Viscosity + Capillarity



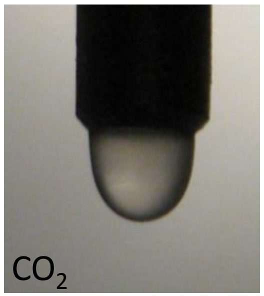
(Modified from Lenormand et al 1988)

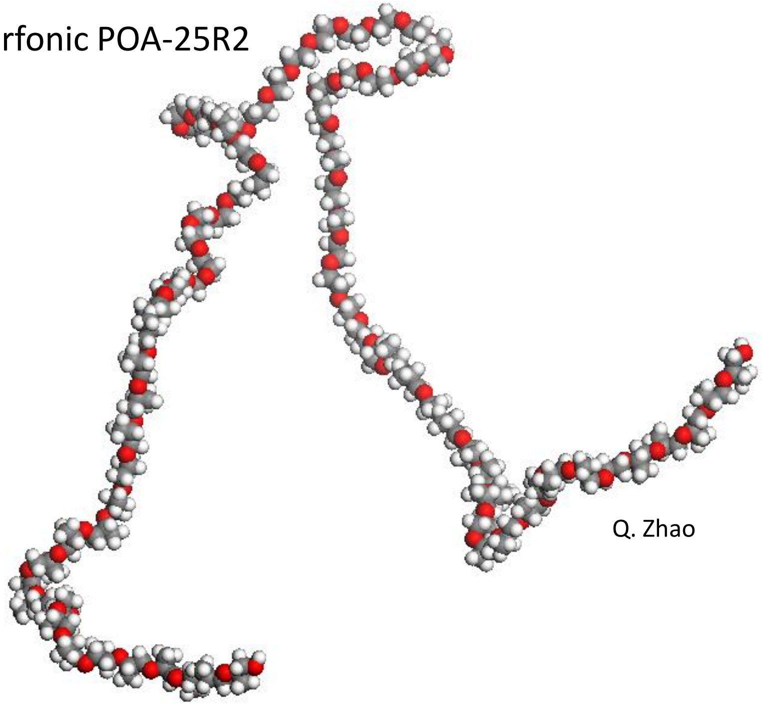
Surfactant

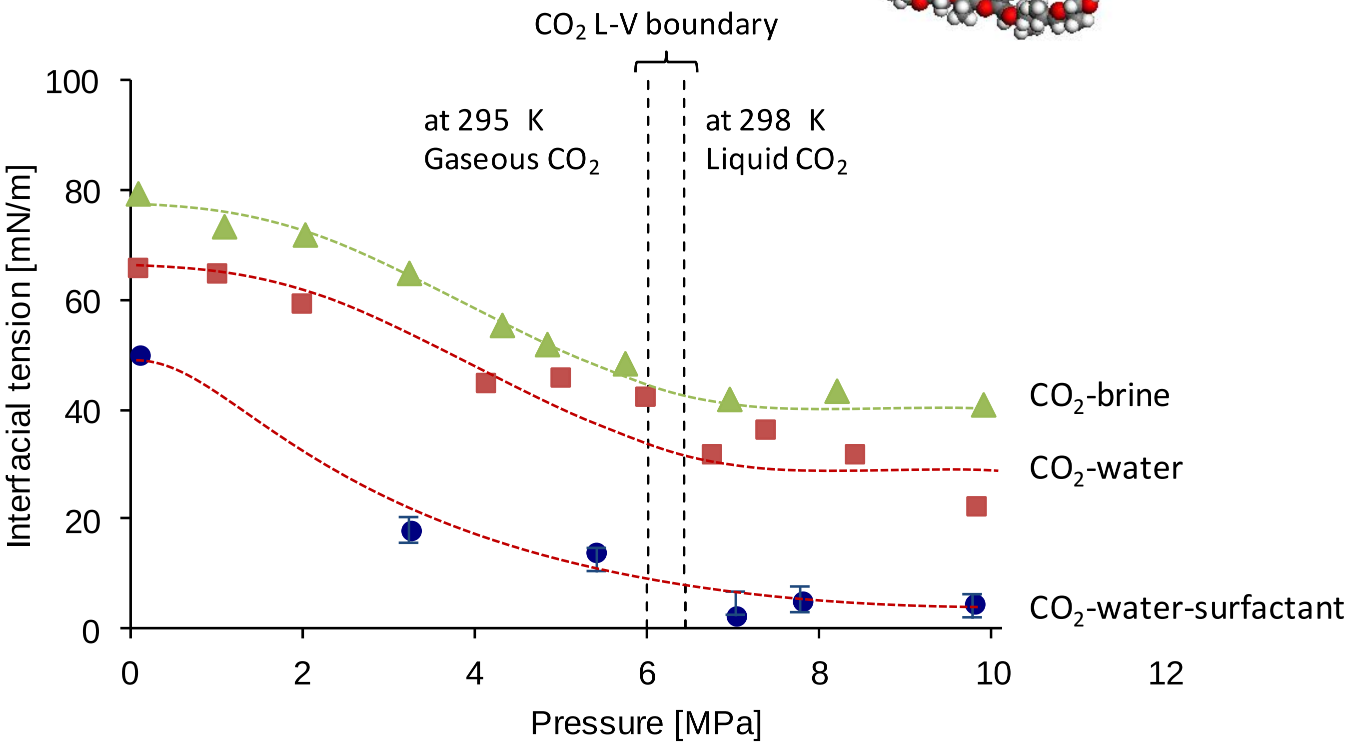
water



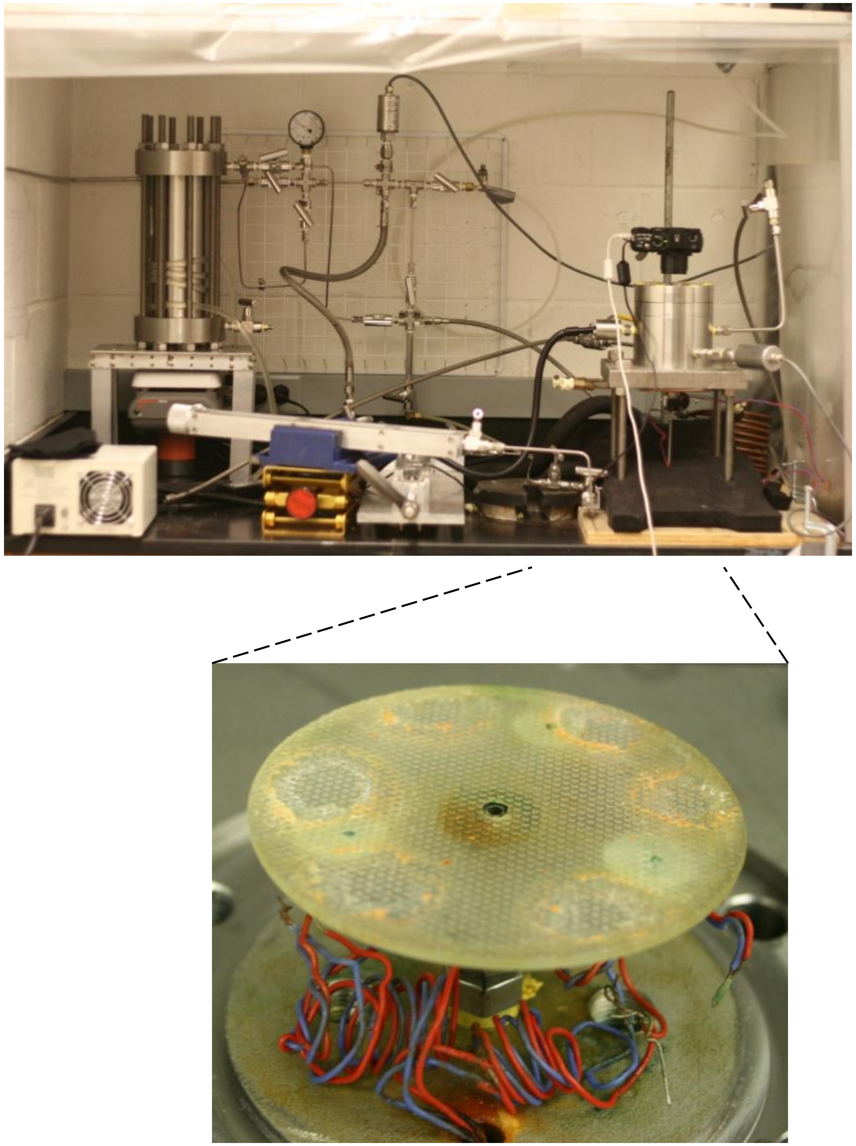
water+surfactant

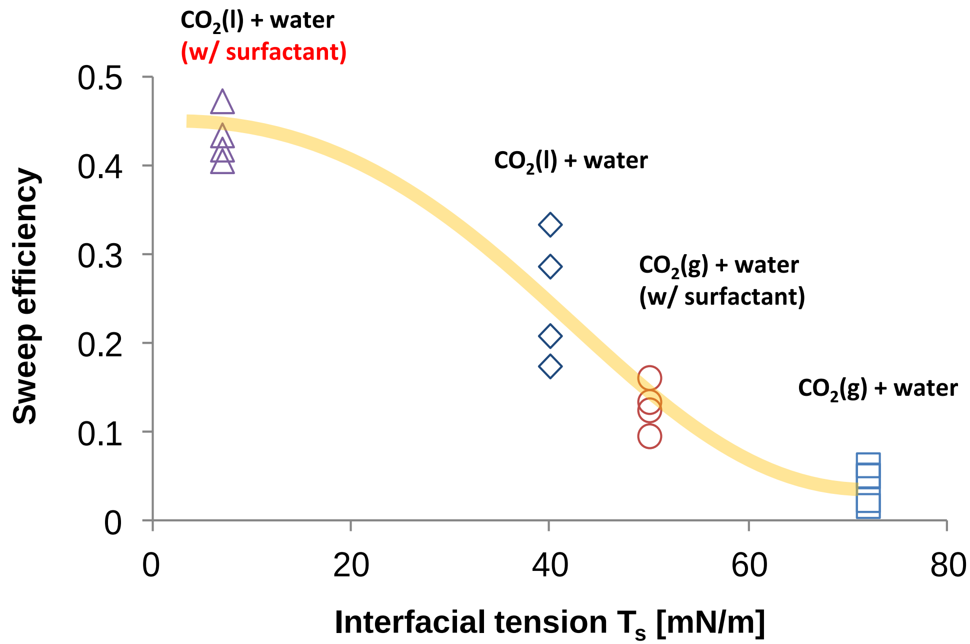


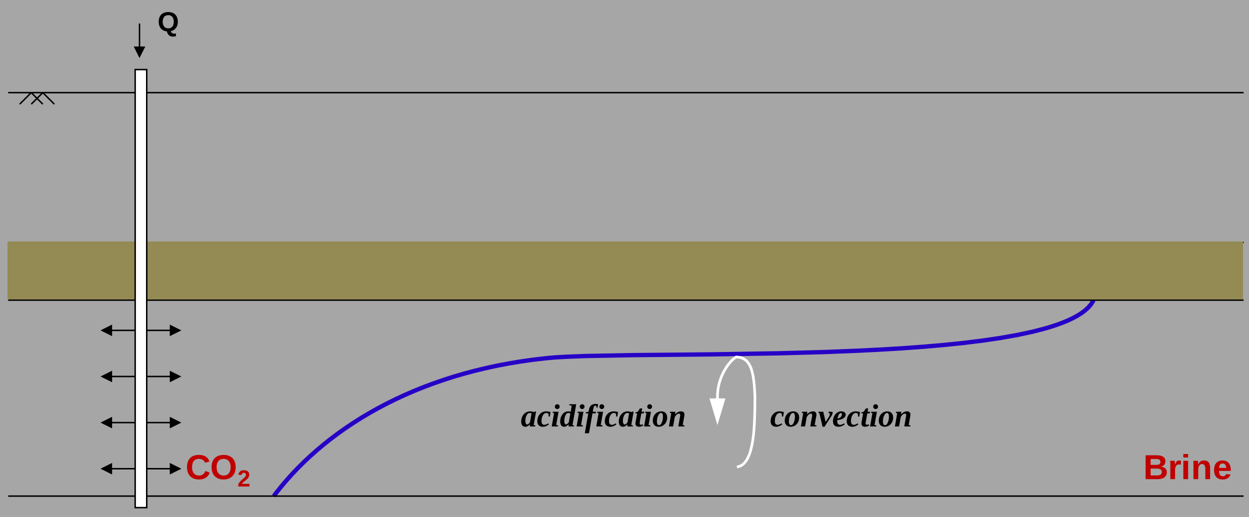




Engineered Injection



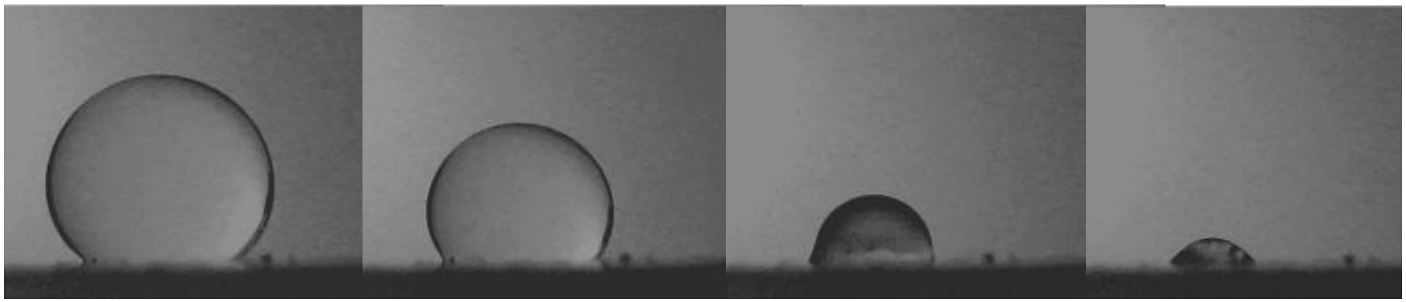




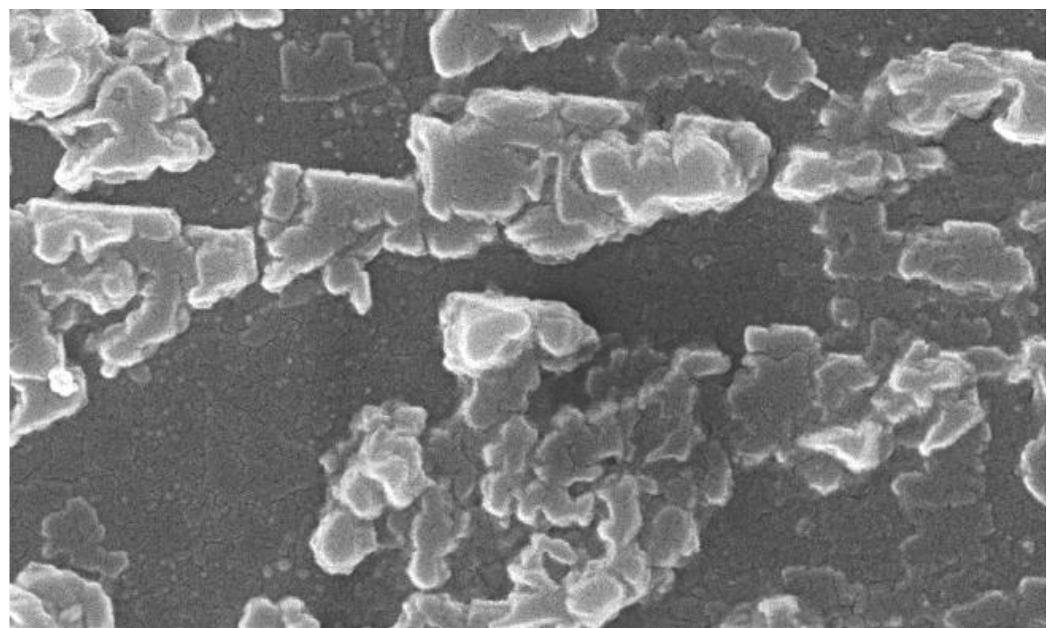
(CO_2 + H_2O) + Mineral

Water in CO_2

acidification → dissolution → drying → precipitation



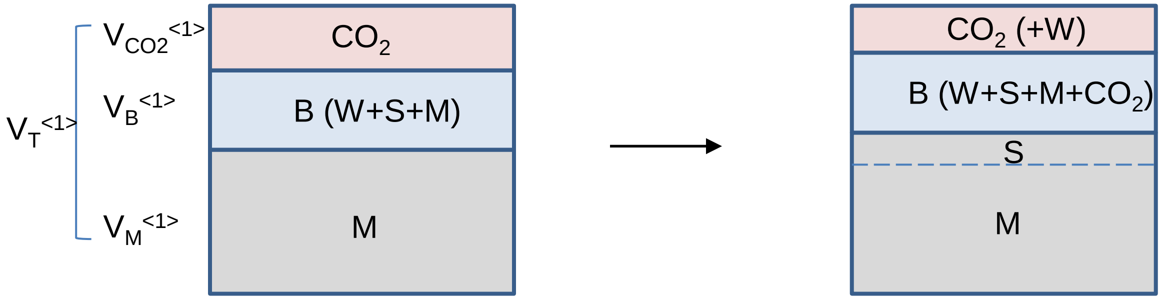
Calcite substrate



Mass Balance Analyses

Volume

At equilibrium:



$$C_W^{CO2} = f(C,P,T)$$
$$C_{CO2}^{B} = f(C,P,T)$$
$$C_M^{B} = f(C,P,T)$$

Concentration

↓

$$\rho_{CO2}^{<2>} = f(C,P,T)$$
$$\rho_{B}^{<2>} = f(C,P,T)$$
$$\rho_{M}^{<2>} = f(C,P,T)$$

Density

Initial porosity: $$\phi^{<1>} = \frac{V_{CO2}^{<1>} + V_B^{<1>}}{V_T^{<1>}}$$

Saturation: $$S_B = \frac{V_B^{<1>}}{V_{CO2}^{<1>} + V_B^{<1>}} \qquad S_{CO2} = 1 - S_B$$

<u>Mass balance</u>:

CO$_2$: $$M_{CO2}^{<1>} = \phi^{<1>} \cdot (1 - S_B) \cdot V_T^{<1>} \cdot \rho_{CO2}^{<1>}$$

Brine: $$M_B^{<1>} = \phi^{<1>} \cdot S_B \cdot V_T^{<1>} \cdot \rho_B^{<1>}$$

Mineral: $$M_M^{<1>} = (1 - \phi^{<1>}) \cdot V_T^{<1>} \cdot \rho_M^{<1>} + C_M^{<1>} \cdot \phi^{<1>} \cdot S_B \cdot V_T^{<1>} \cdot \rho_B^{<1>}$$

Salt: $$M_S^{<1>} = C_S^{<1>} \cdot \phi^{<1>} \cdot S_B \cdot V_T^{<1>} \cdot \rho_B^{<1>}$$

$=$

$$M_{CO2}^{T} = M_{CO2}^{CO2} + M_{CO2}^{B}$$
$$M_B^{T} = M_B^{B} + M_W^{CO2}$$
$$M_M^{T} = M_M^{M} + M_M^{B}$$
$$M_S^{T} = M_S^{S} + M_S^{B}$$

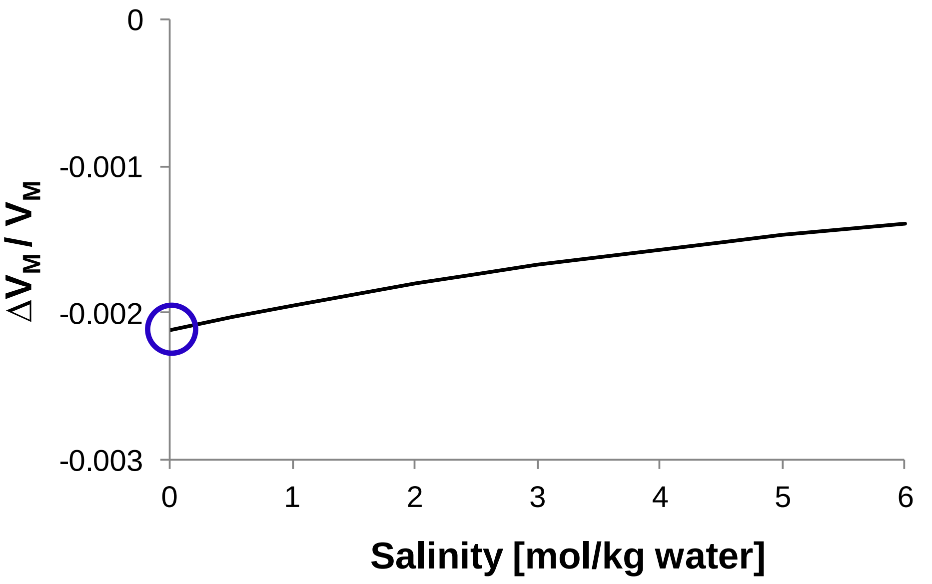
→

Final volume

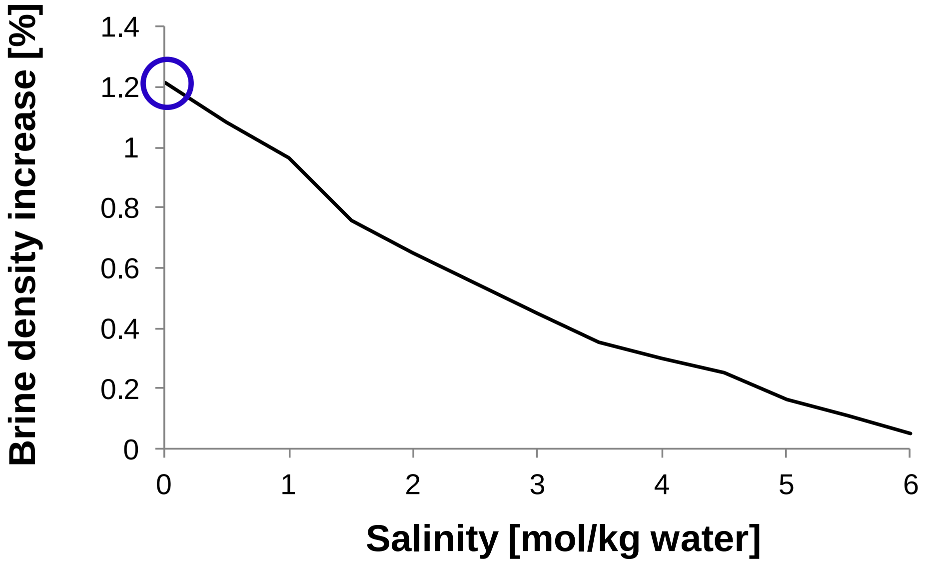
$$V_{CO2}^{<2>} = \frac{M_{CO2}^{<2>}}{\rho_{CO2}^{<2>}}$$
$$V_B^{<2>} = \frac{M_B^{<2>}}{\rho_B^{<2>}}$$
$$V_M^{<2>} = \frac{M_M^{<2>}}{\rho_M^{<2>}}$$

Mineral Dissolution

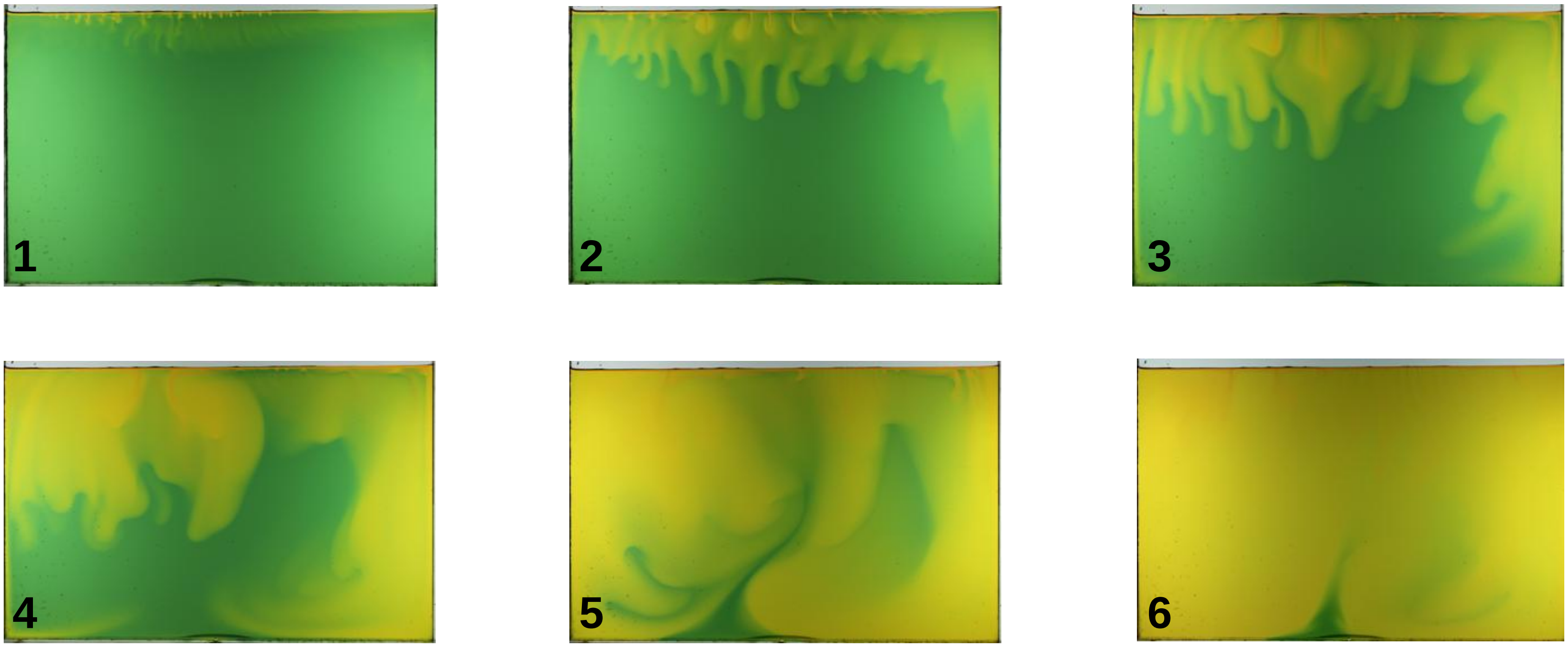
Normalized change in mineral volume
≤ 0.2%



Increase in brine density
≤ 1.2%



Convection



Convection time

$$t_{conv} = \frac{\mu \, H_R}{k \; \Delta\gamma}$$

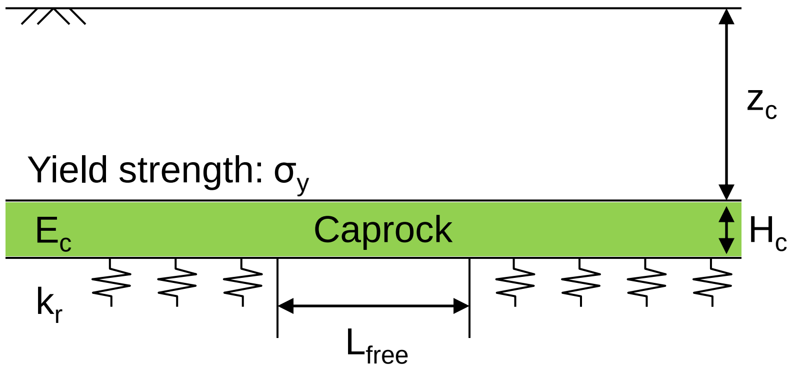
Case: k= 200 md H_R=10 m

$t_{conv} \approx$ 9years

Bending Failure in Caprock

Maximum tensile stress σ_{tmax}:

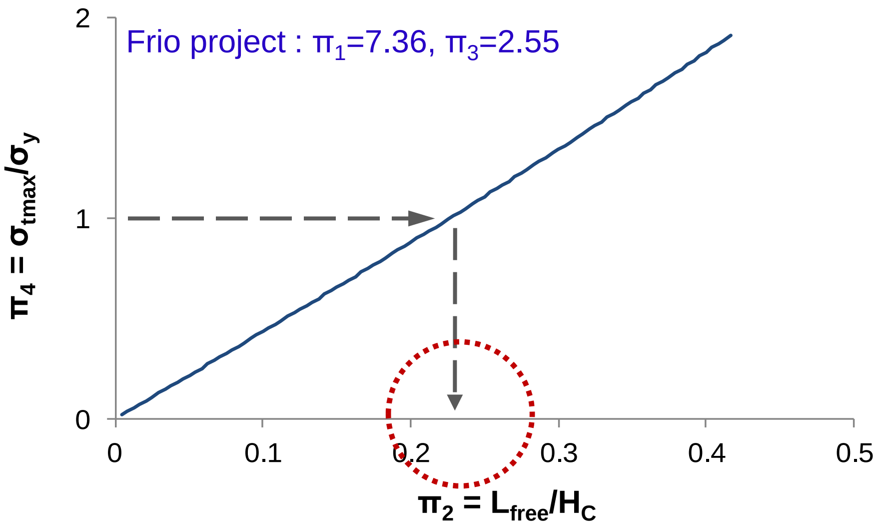
$$\frac{\sigma_{tmax}}{\sigma_y} = 3\pi_1\pi_2\left\{\frac{1}{4}\pi_2 + \frac{6-(\pi_2\pi_3)^2}{6\pi_3(2+\pi_2\pi_3)}\right\}$$



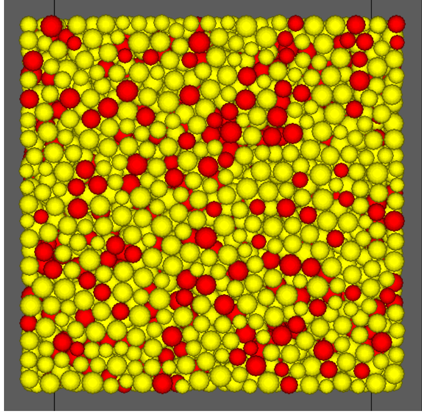
where:

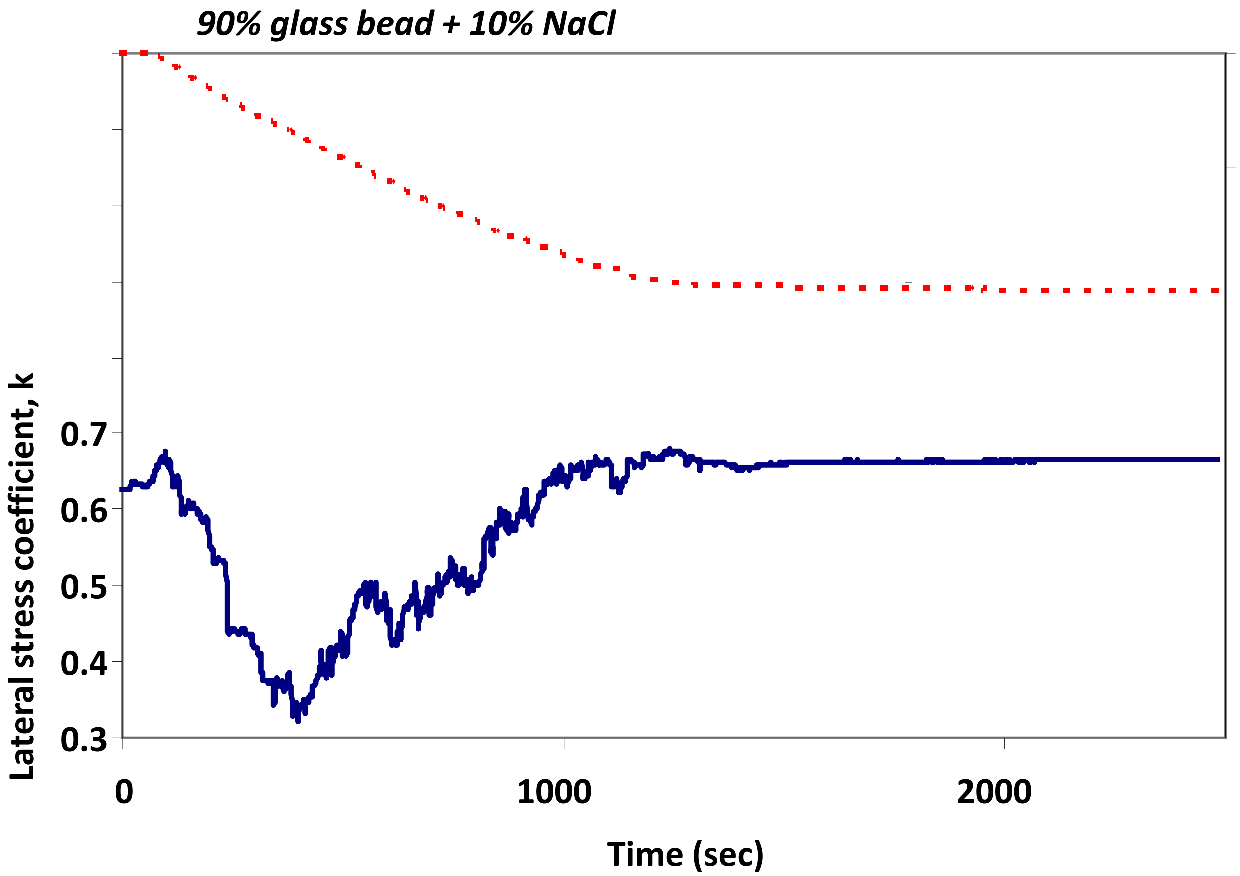
$$\pi_1 = \frac{\gamma_c z_c}{\sigma_y} \qquad \pi_2 = \frac{L_{free}}{H_c}$$

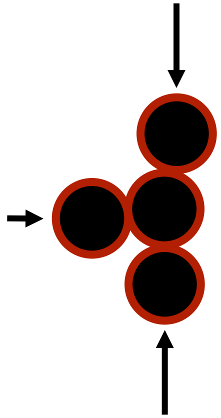
$$\pi_3 = \lambda H_c \qquad \lambda = \sqrt[4]{\frac{k_r}{4E_cI_c}}$$



Mineral Dissolution - Implications

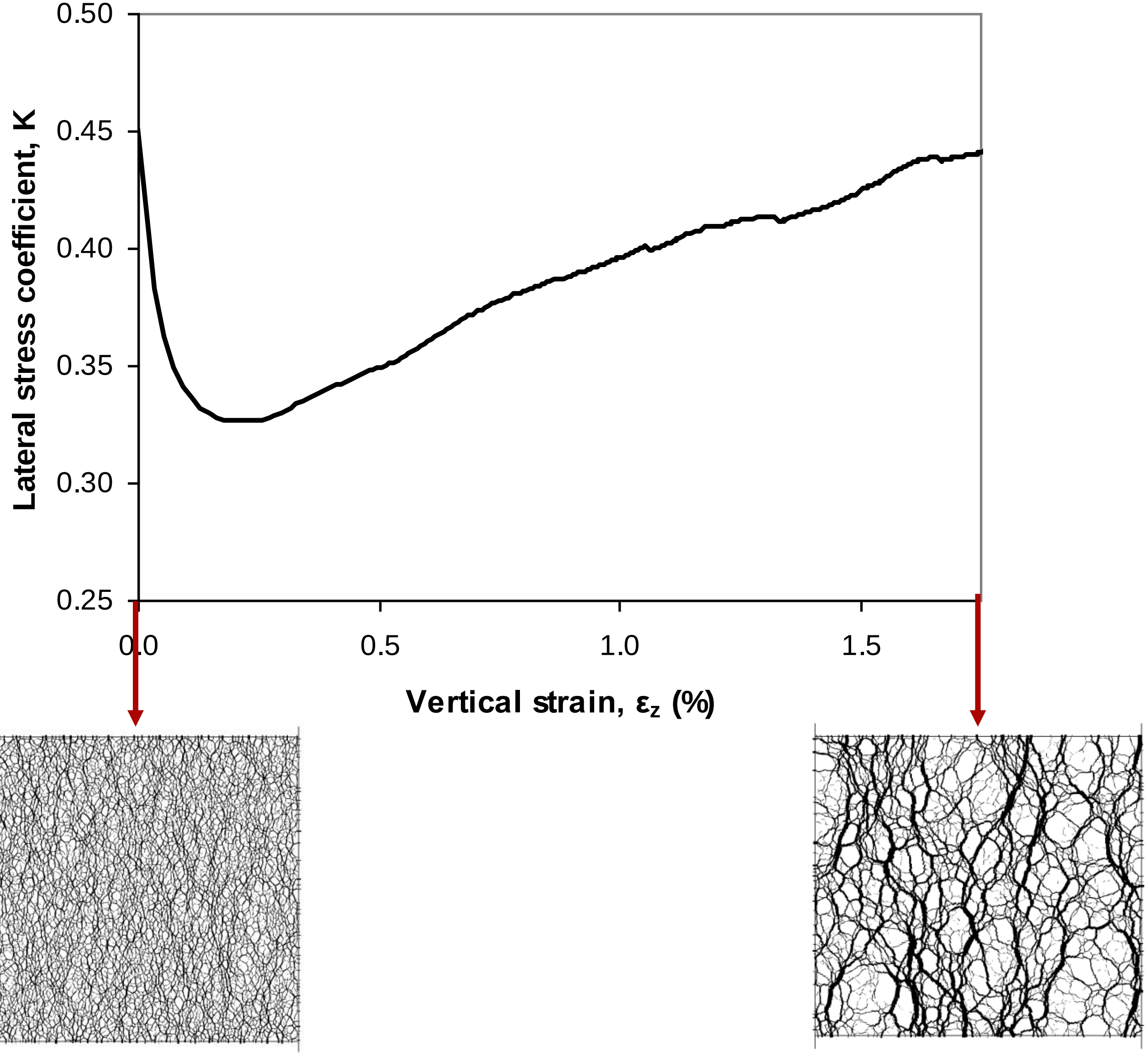




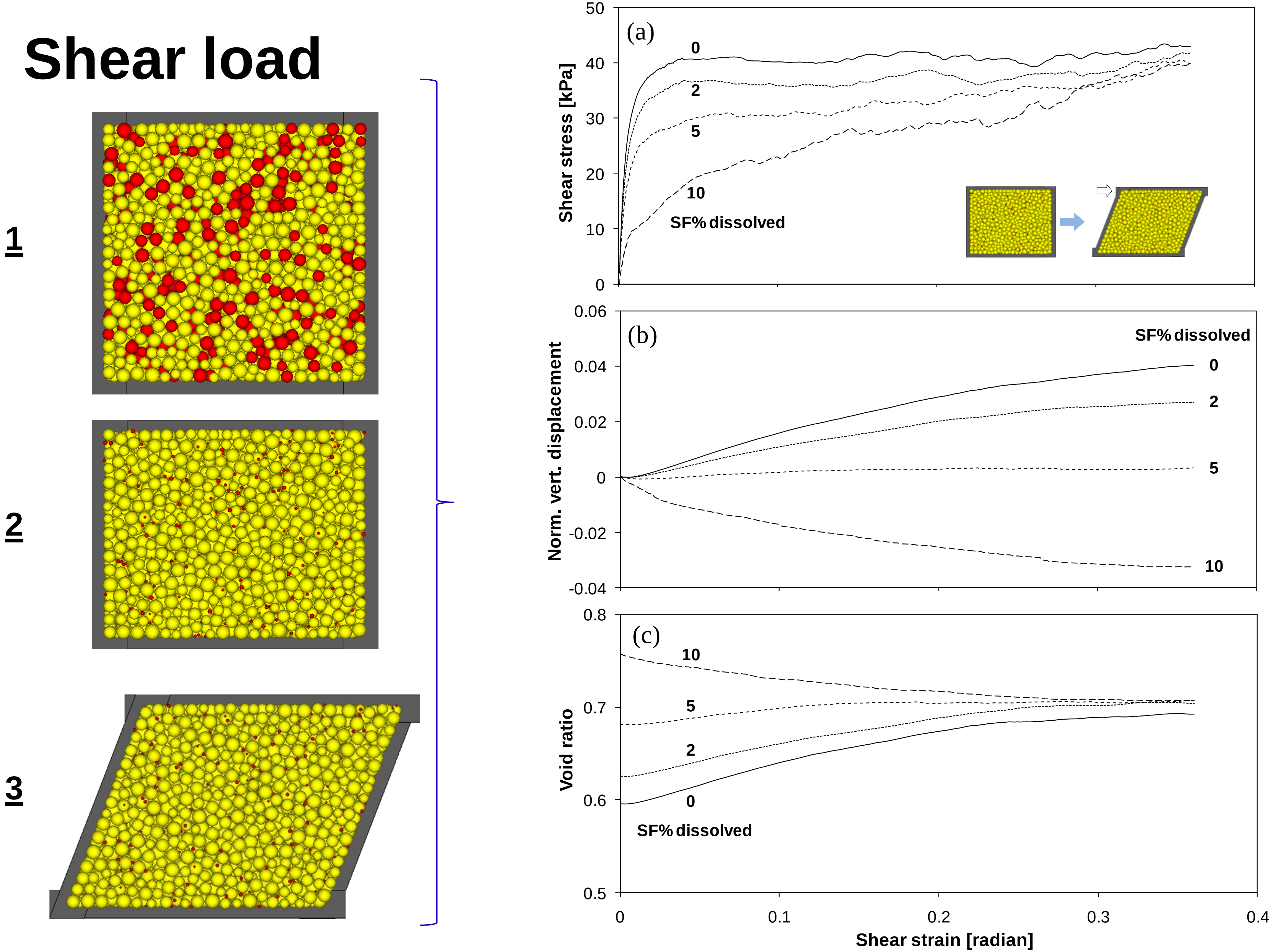


DEM Simulation

2D - diameter gradually reduced - 20% of particles



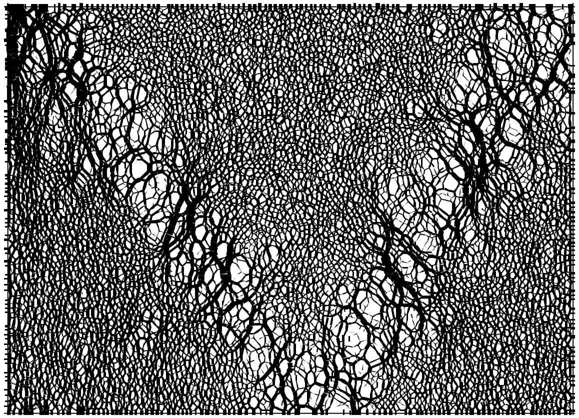
Shear load



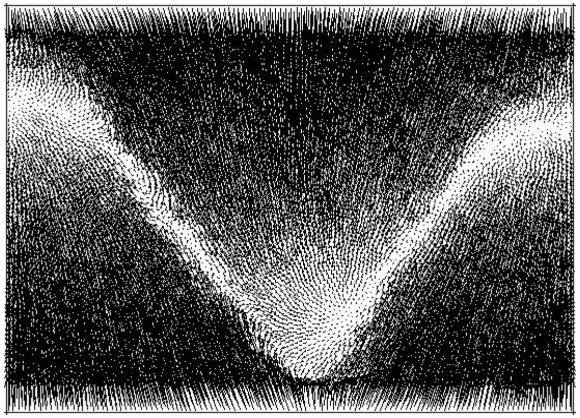
1
2
3
(a)
Shear stress [kPa]
50
40
30
20
10
0
0
2
5
10
SF% dissolved
(b)
Norm. vert. displacement
0.06
0.04
0.02
0
-0.02
-0.04
SF% dissolved
0
2
5
10
(c)
Void ratio
0.8
0.7
0.6
0.5
10
5
2
0
SF% dissolved
0
0.1
0.2
0.3
0.4
Shear strain [radian]

Emergent: Shear Localization

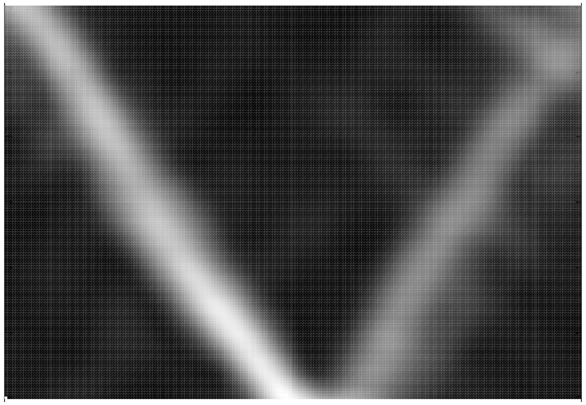
Contact Force Chains

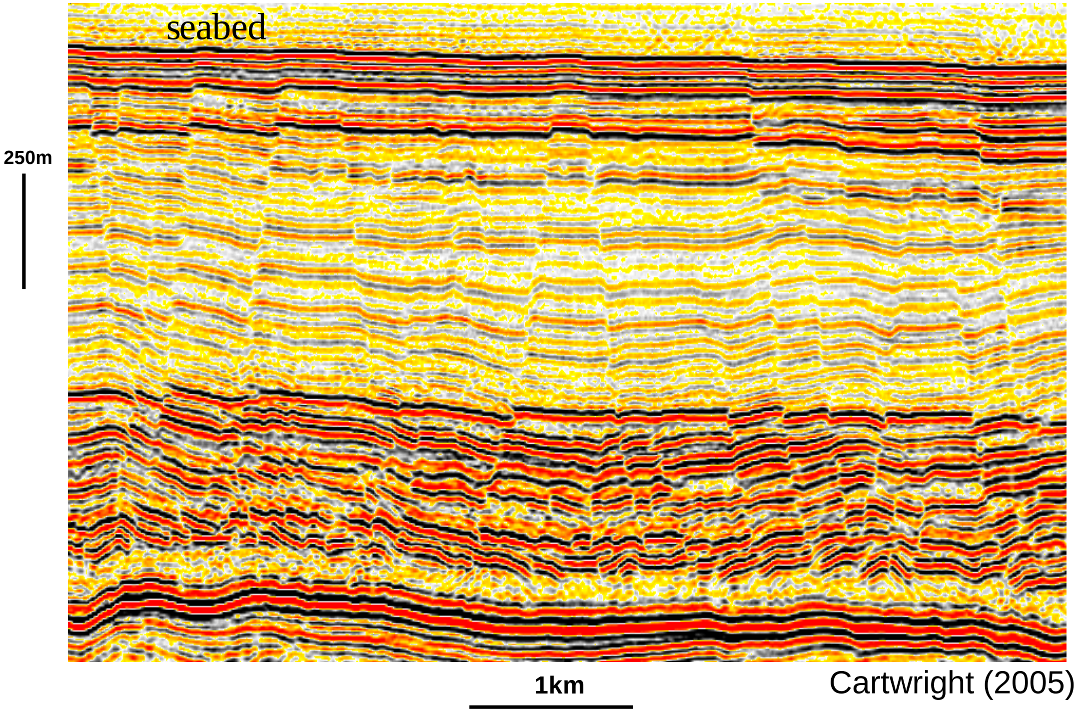


Displacement vectors



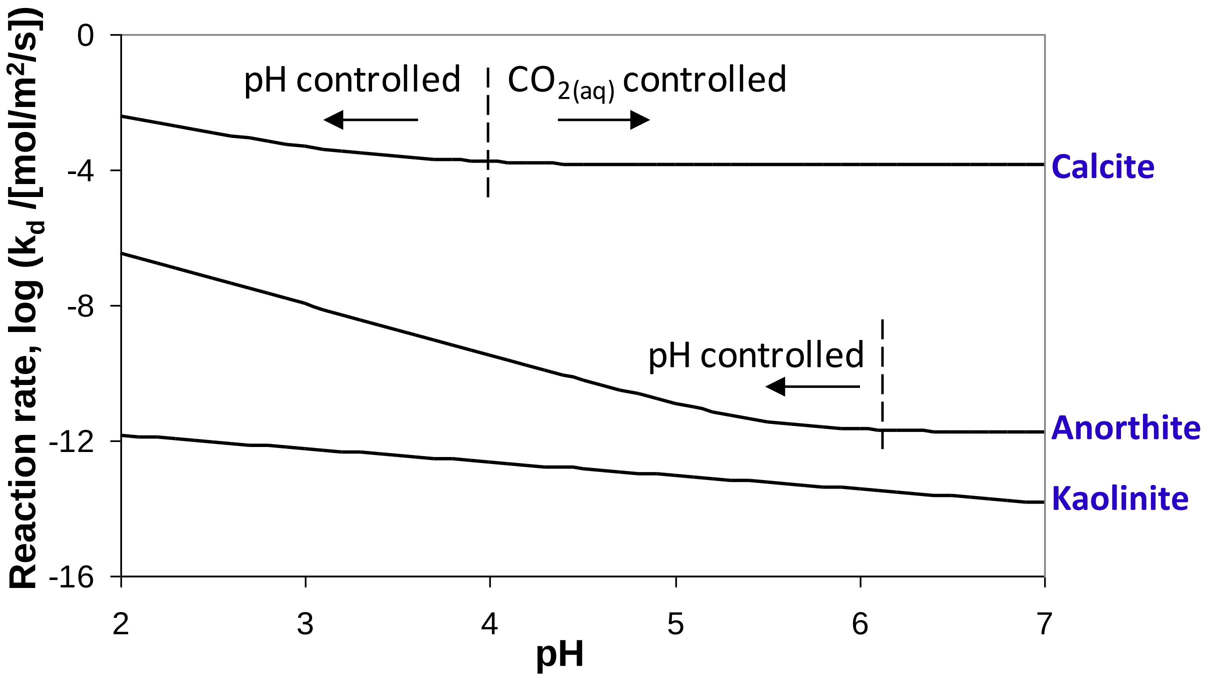
Strain field





Cartwright (2005)

Dissolution Rate



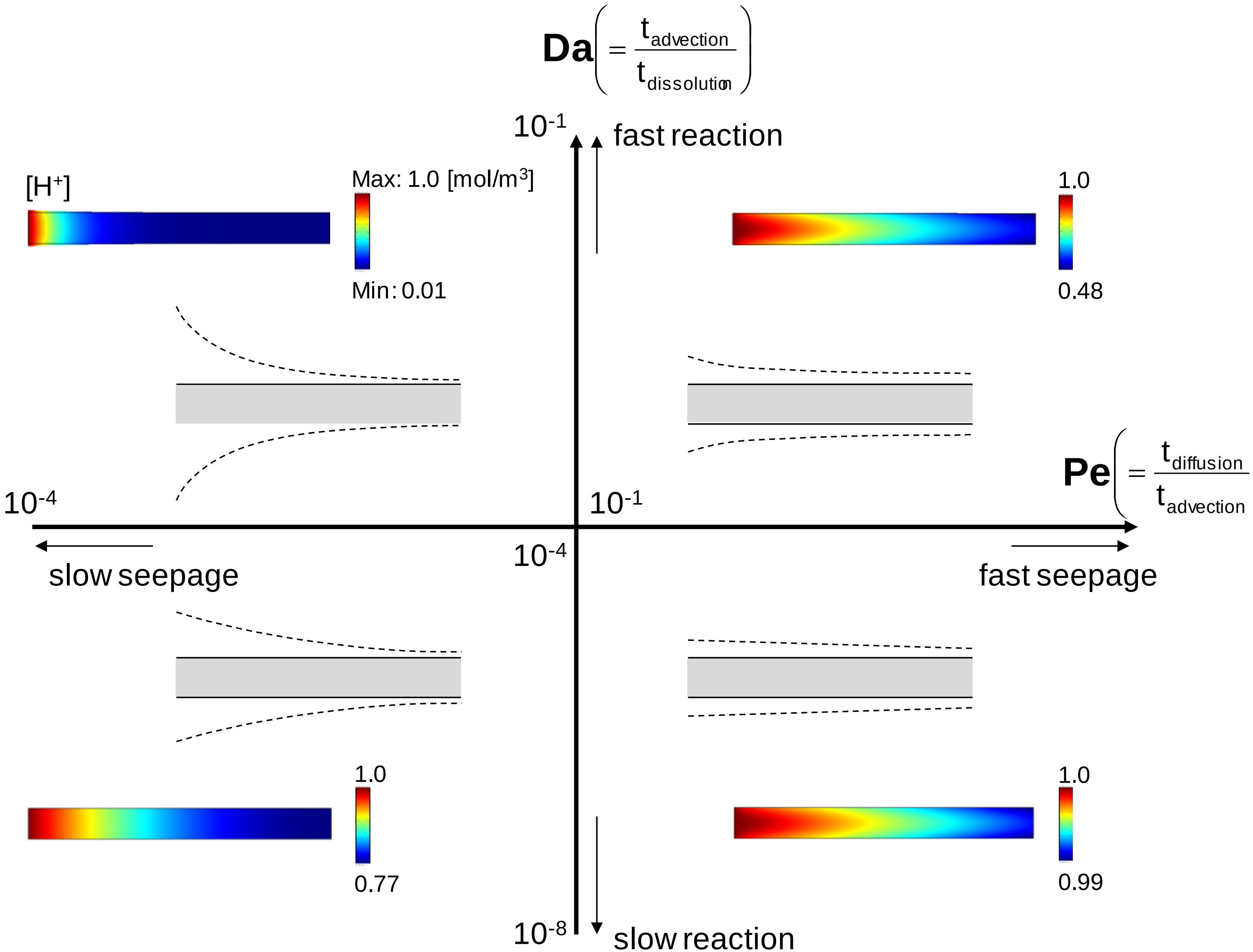
Calcite: $$k_d = k_1[H^+] + k_2[CO_{2(aq)}]$$

Anorthite: $$k_d = k_H[H^+]^{1.5} + k_{H2O} + k_{OH}[OH^-]^{0.33}$$

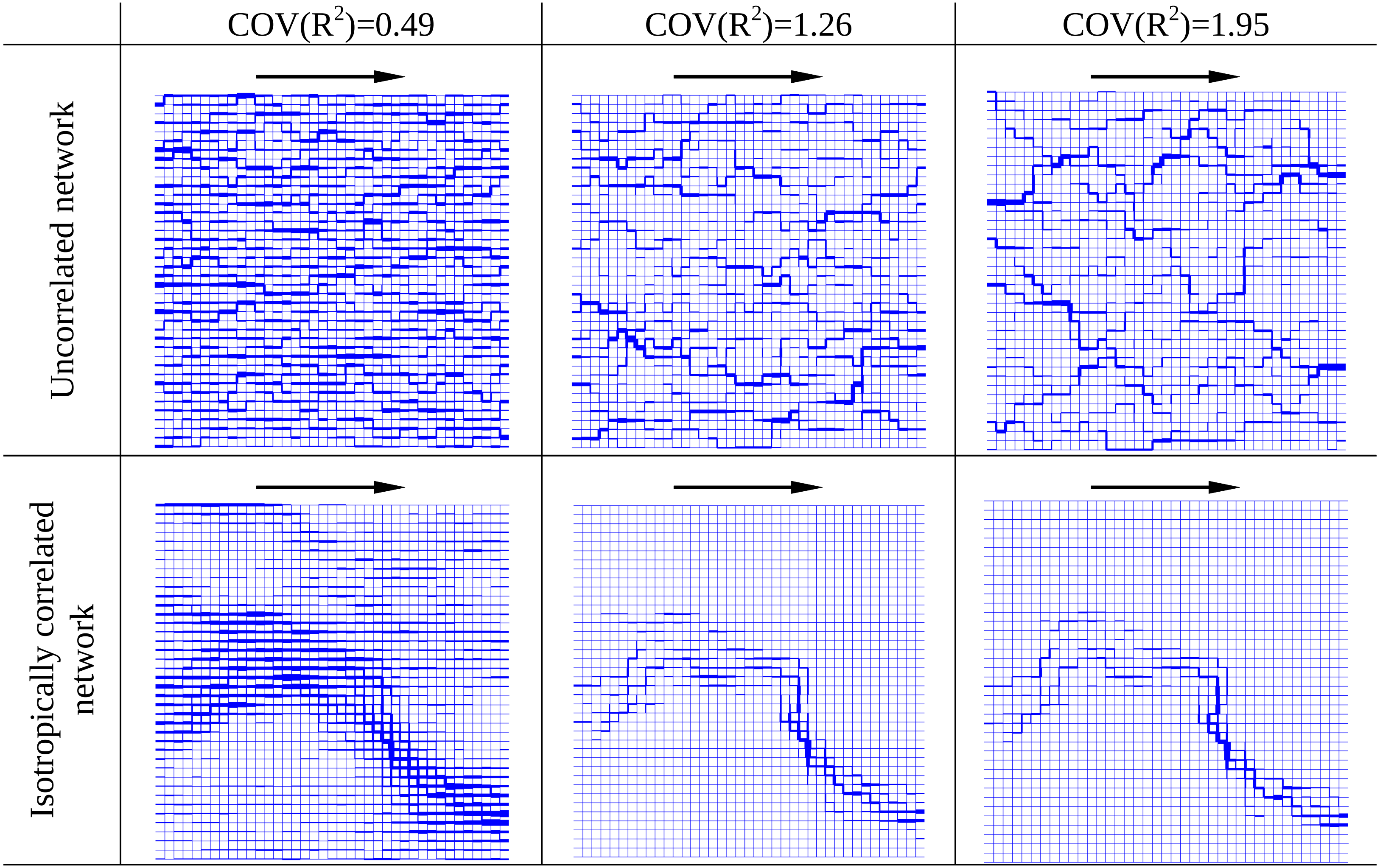
Kaolinite: $$k_d = k_H[H^+]^{0.4} + k_{OH}[OH^-]^{0.3}$$

Calcite: Fredd and Fogler, 1998 & Renard et al., 2005 Anorthite & Kaolinite: Li et al., 2006

Single Rock Joint / Pore Scale (FEM)

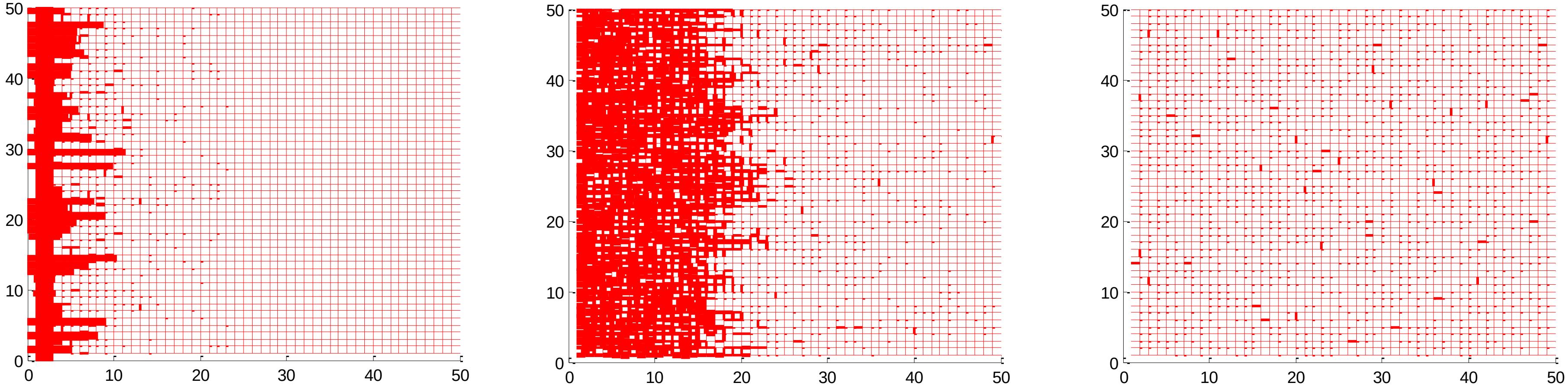


Network Simulation: Non-Reactive

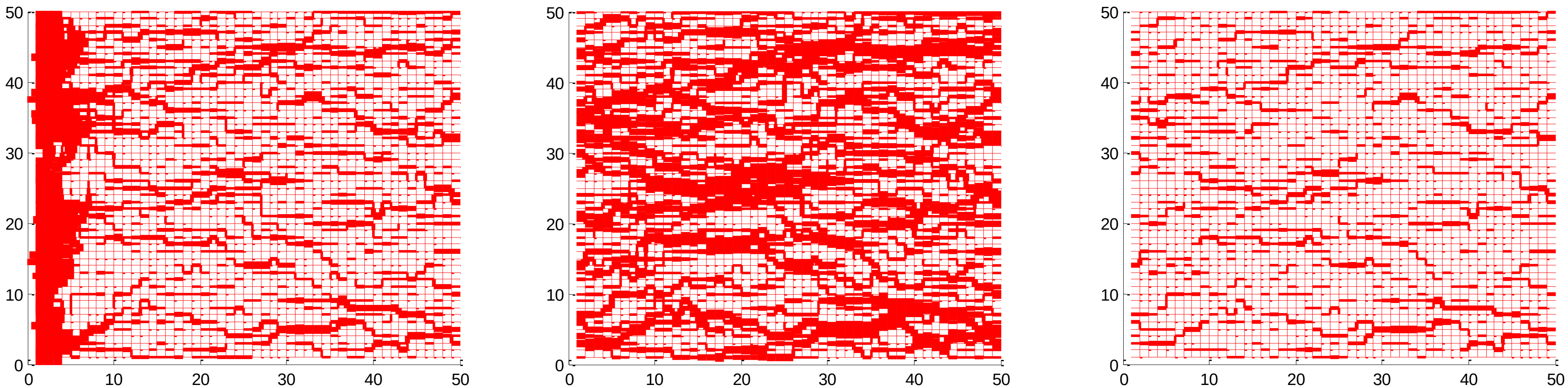


Network Simulation: Storage Reservoir

Normalized change in tube diameter $\Delta d/d_0$

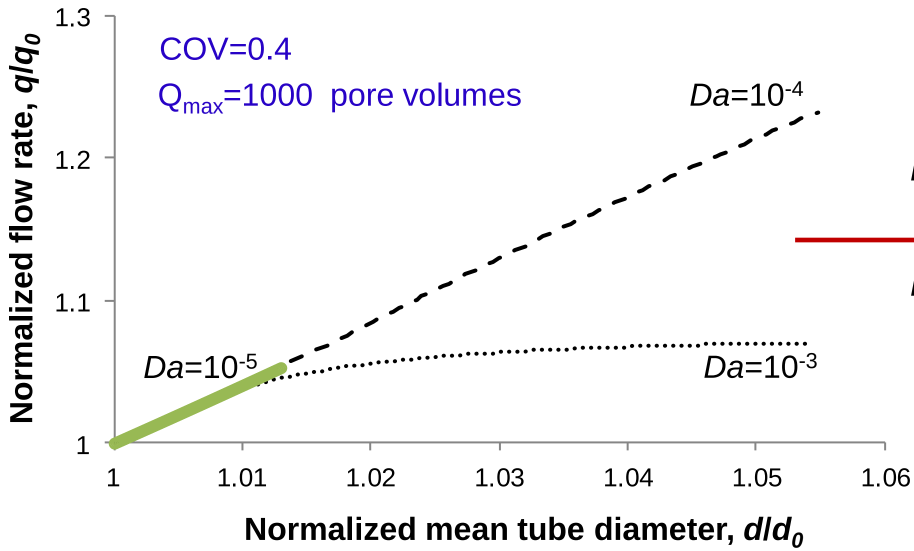


Normalized change in flow rate $\Delta q/\Delta q_{0,max}$



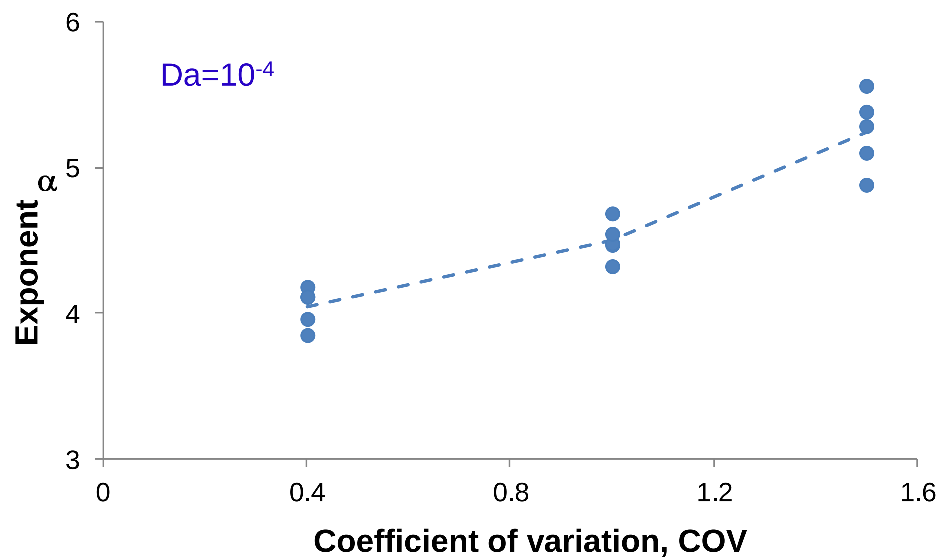
(a) Da~10^{-3} (i_h=10) (b) Da~10^{-4} (i_h=100) (c) Da~10^{-5} (i_h=1000)

Mean Pore Diameter and Flow Rate



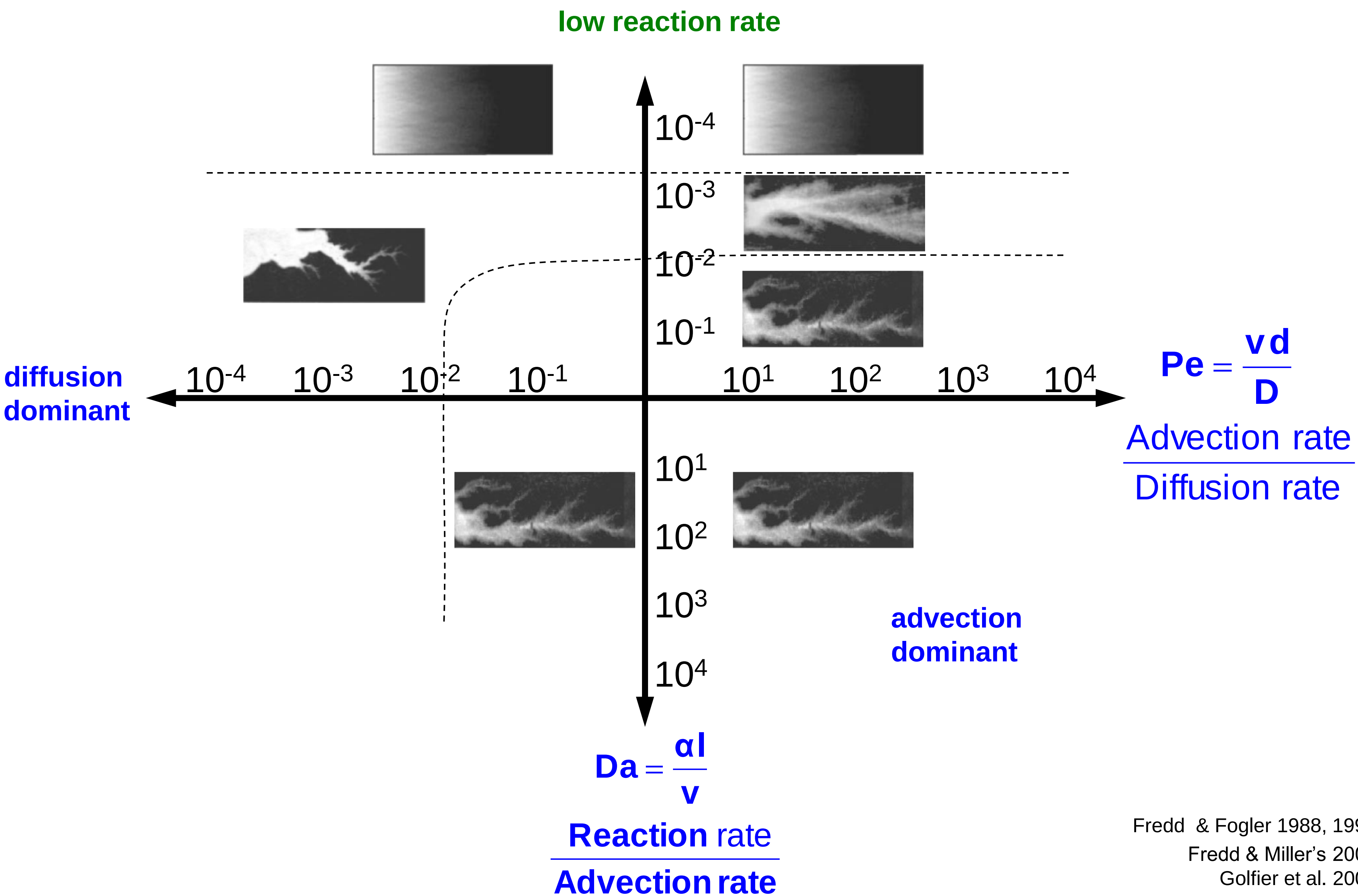
***Da*≤10^{-4}: several branches of localized flow**

***Da*>10^{-4}: evolves towards compact dissolution**



$$\frac{q}{q_0} = \left(\frac{d}{d_0}\right)^{\alpha}$$

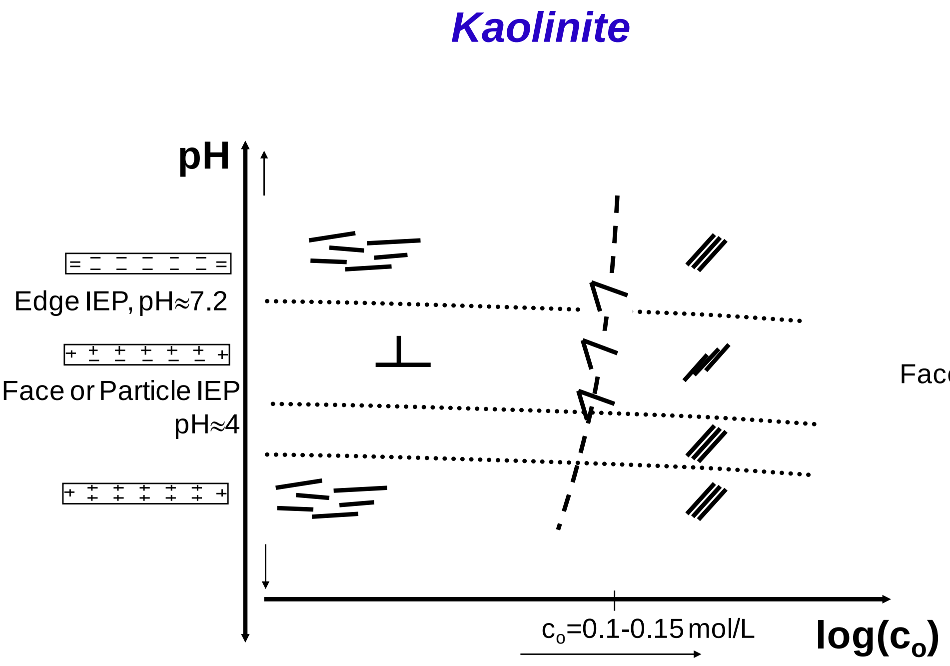
Reactive Fluid Transport



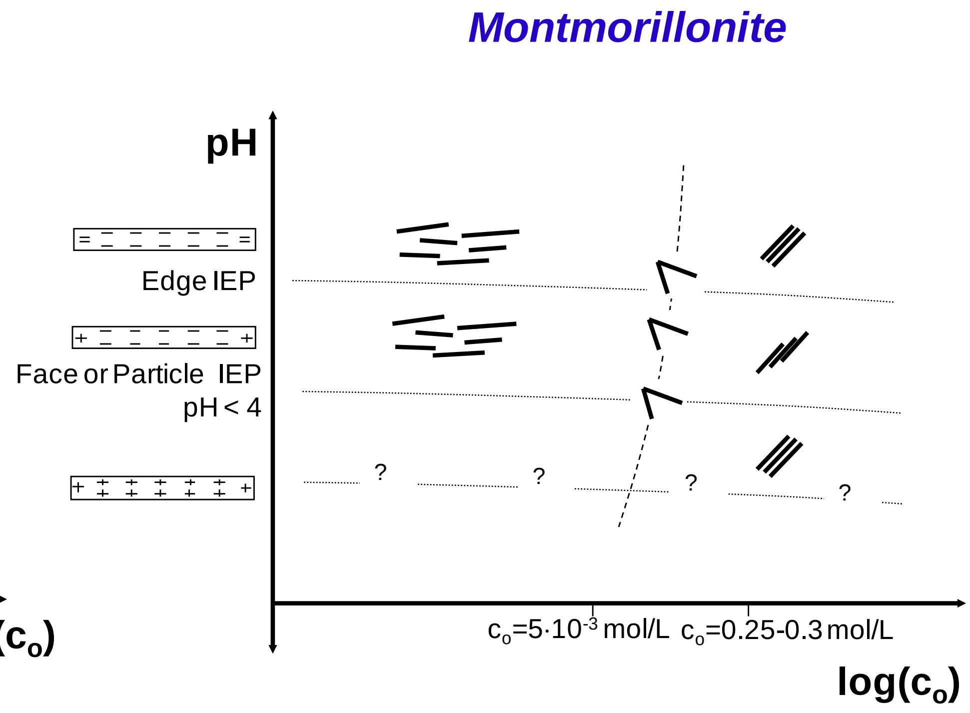
Fredd & Fogler 1988, 1998
Fredd & Miller's 2000
Golfier et al. 2002

(water, CO_2) + clay minerals

Fabric map

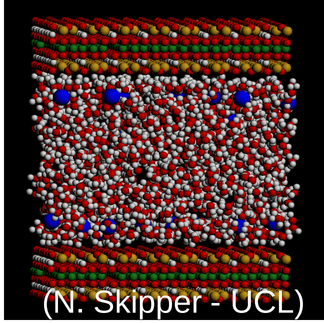


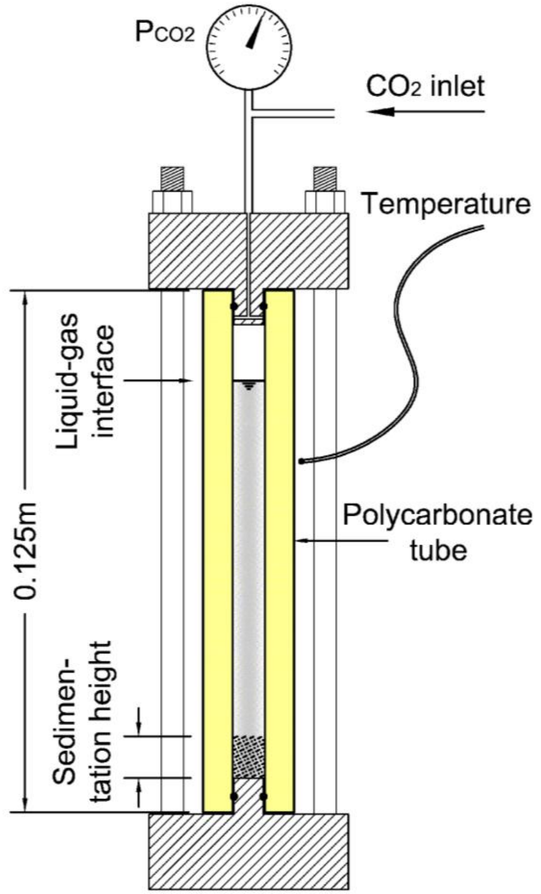
Kaolinite
pH
Edge IEP, pH≈7.2
Face or Particle IEP
pH≈4
c$_o$=0.1-0.15 mol/L
log(c$_o$)



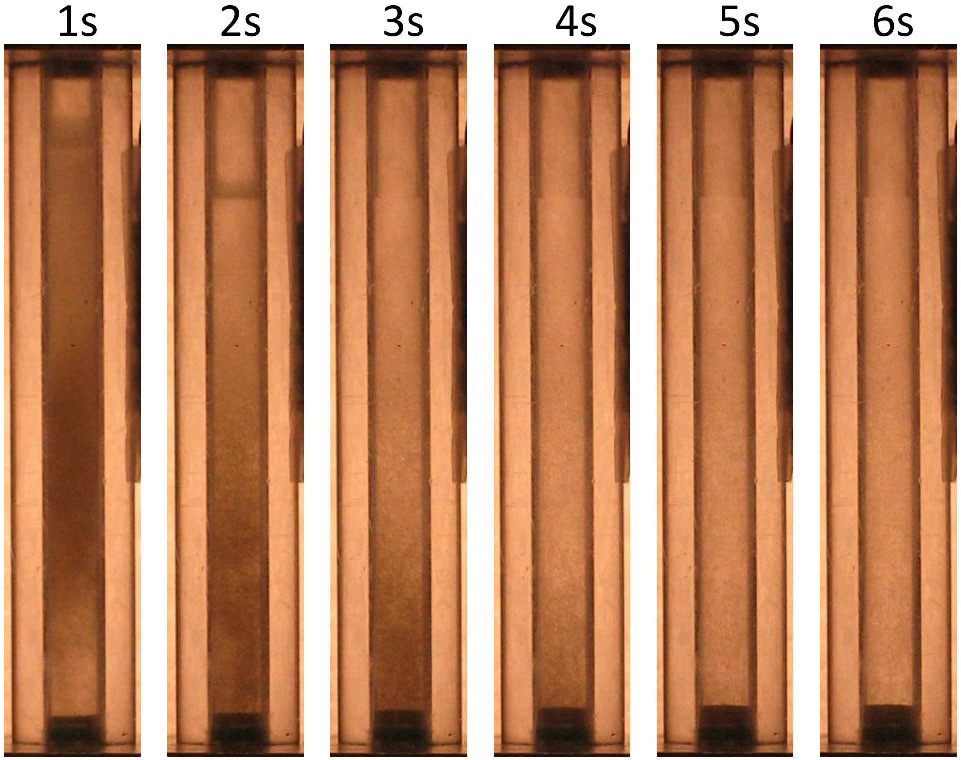
Montmorillonite
pH
Edge IEP
Face or Particle IEP
pH < 4
?
?
?
?
c$_o$=5·10^{-3} mol/L
c$_o$=0.25-0.3 mol/L
log(c$_o$)

Clay-CO_2 interaction

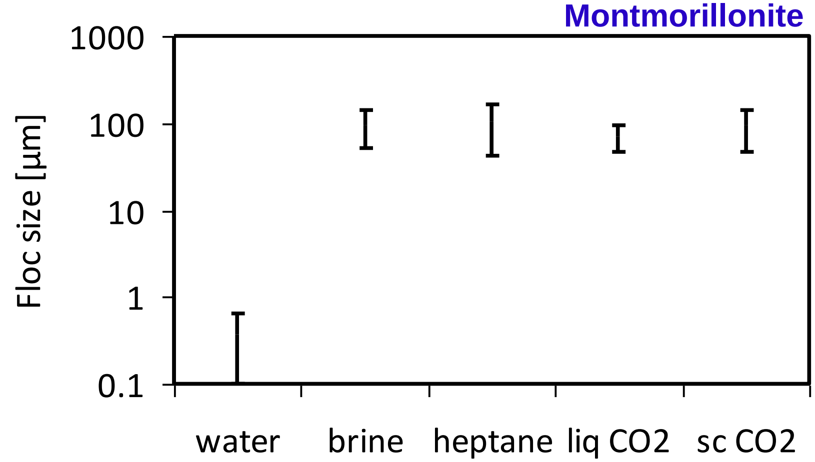


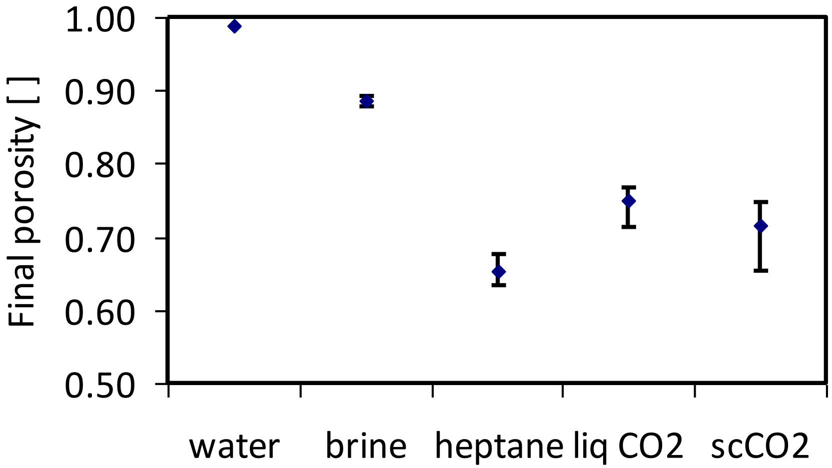


montmorillonite in liquid CO_2



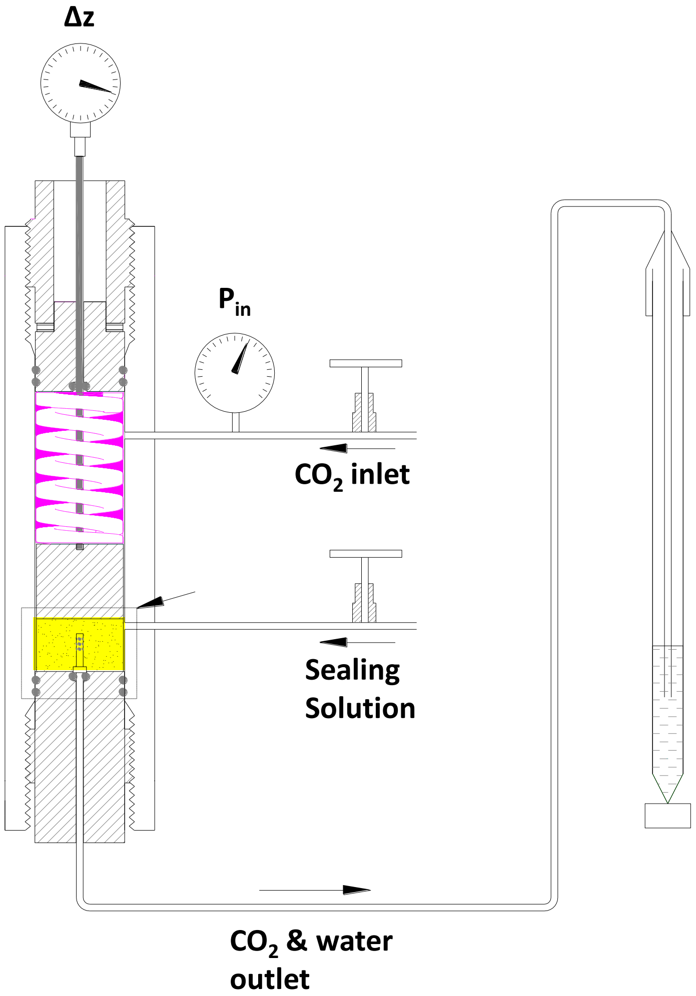
Clay-CO_2 interaction

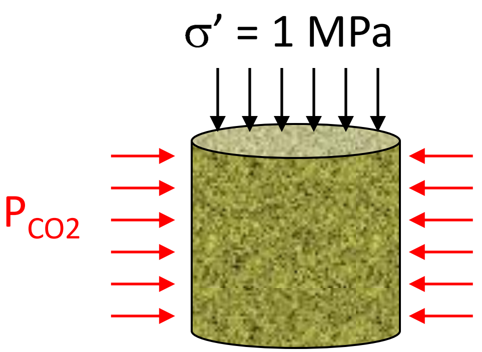




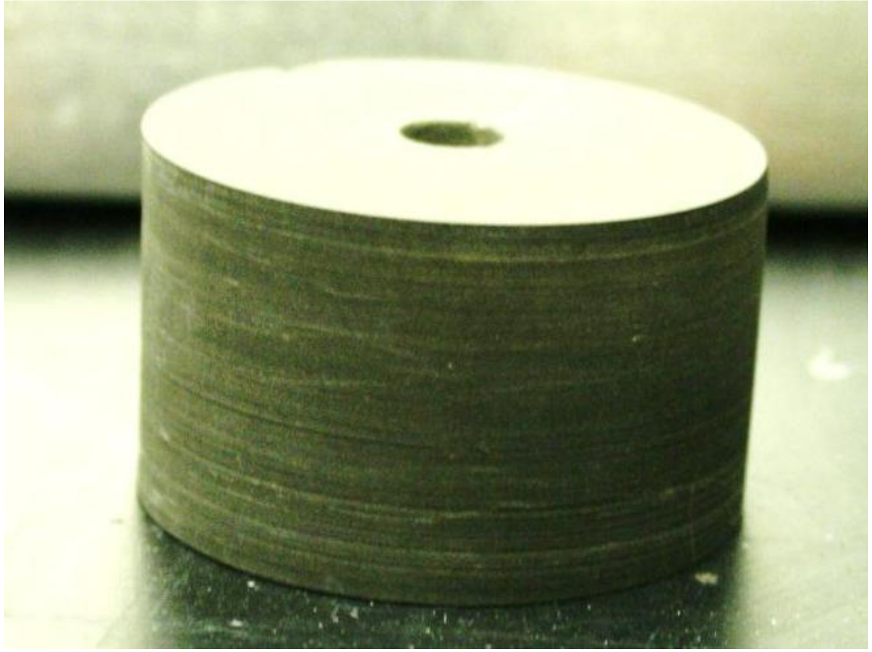
κ'	78.5	56	1.385	1.167	1.167
A_H	0.98	0.73	0.42	3.14	3.14

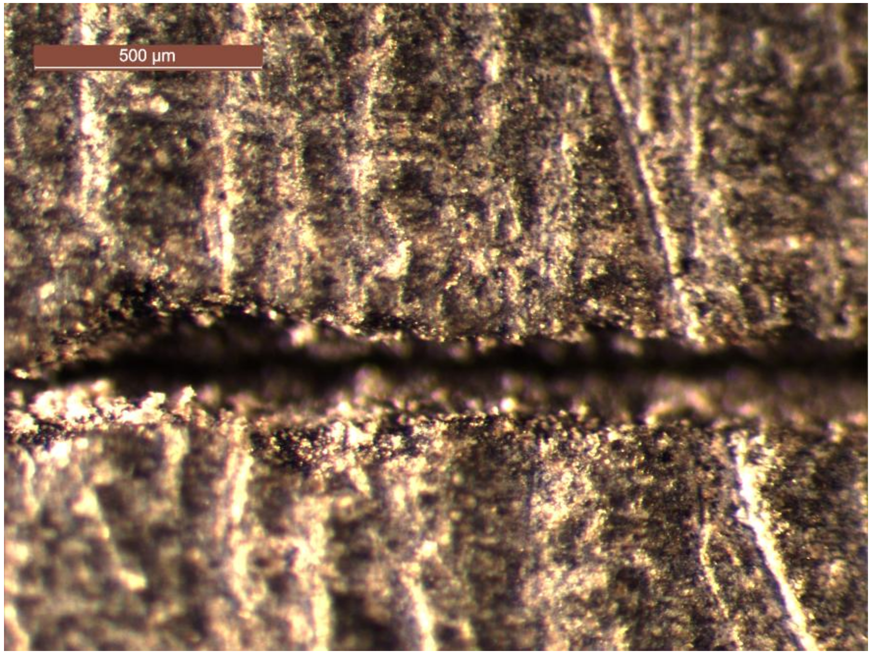
Breakthrough – Healing (self-healing?)





Caprock: Chattanooga Shale





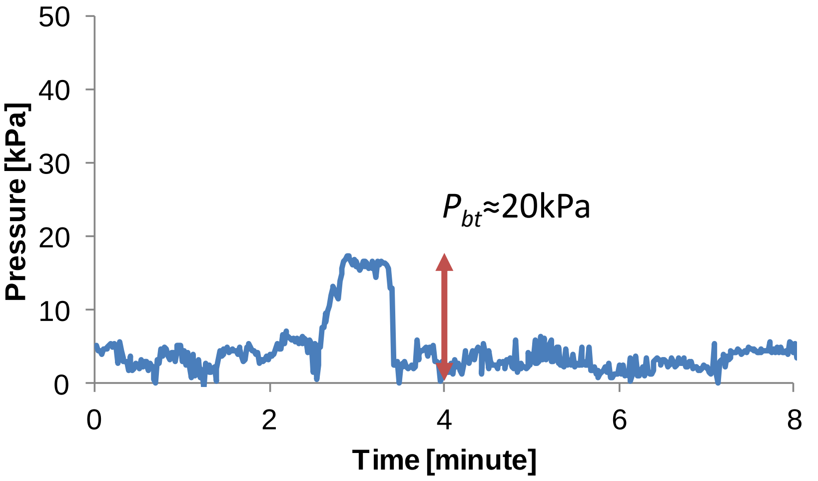
OD= 40mm

ID= 3.17mm

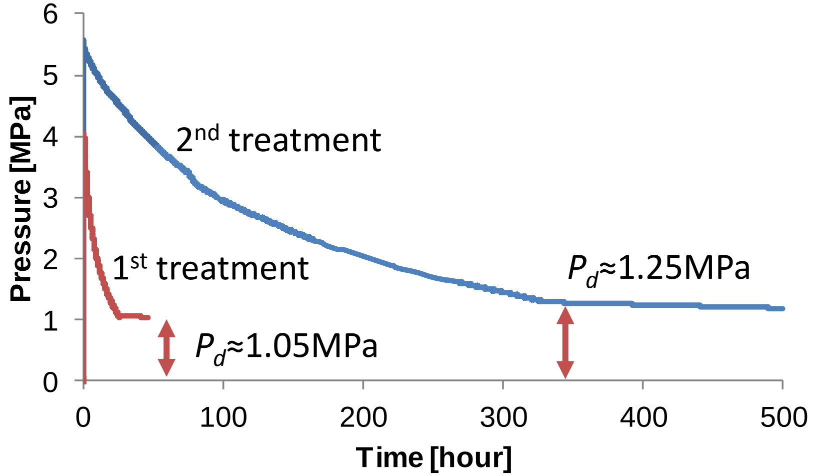
Height: 25mm<*h*<35mm

Caprock: Chattanooga Shale

Initial breakthrough test

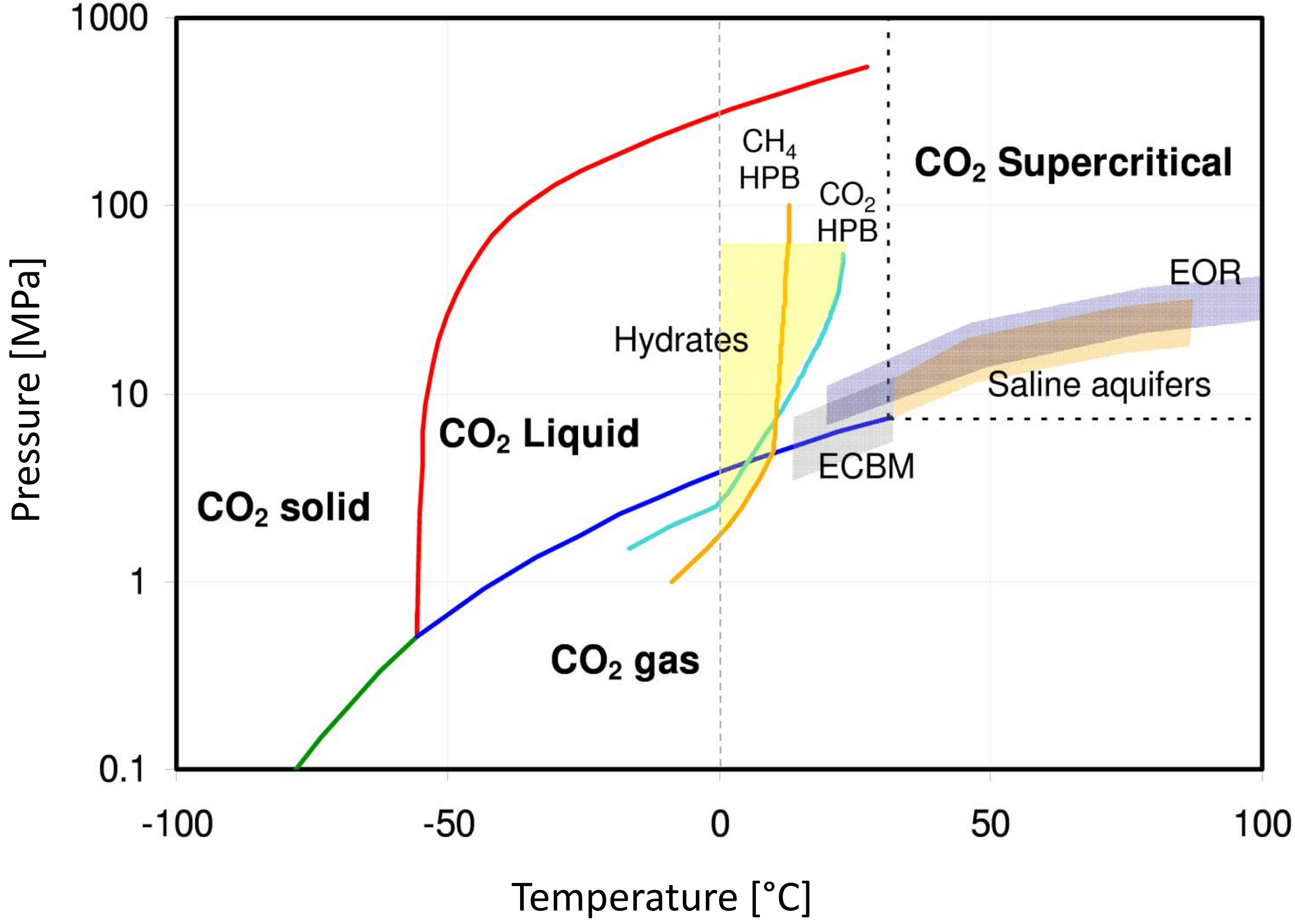


After sealing treatments

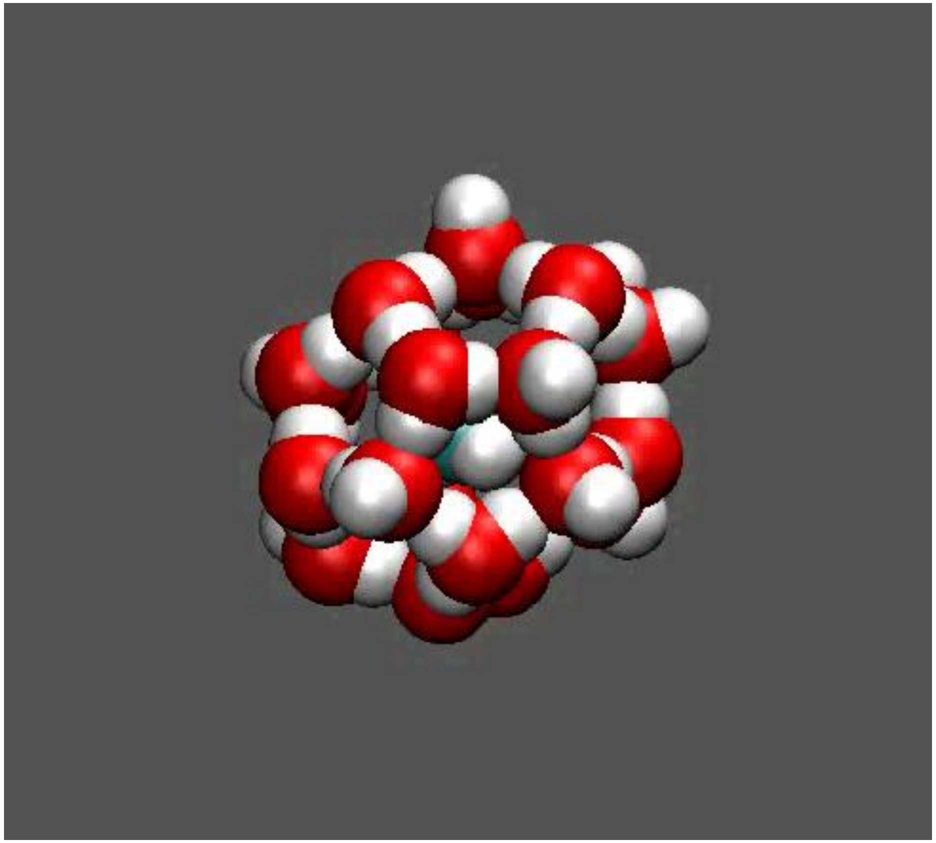


Hydrates

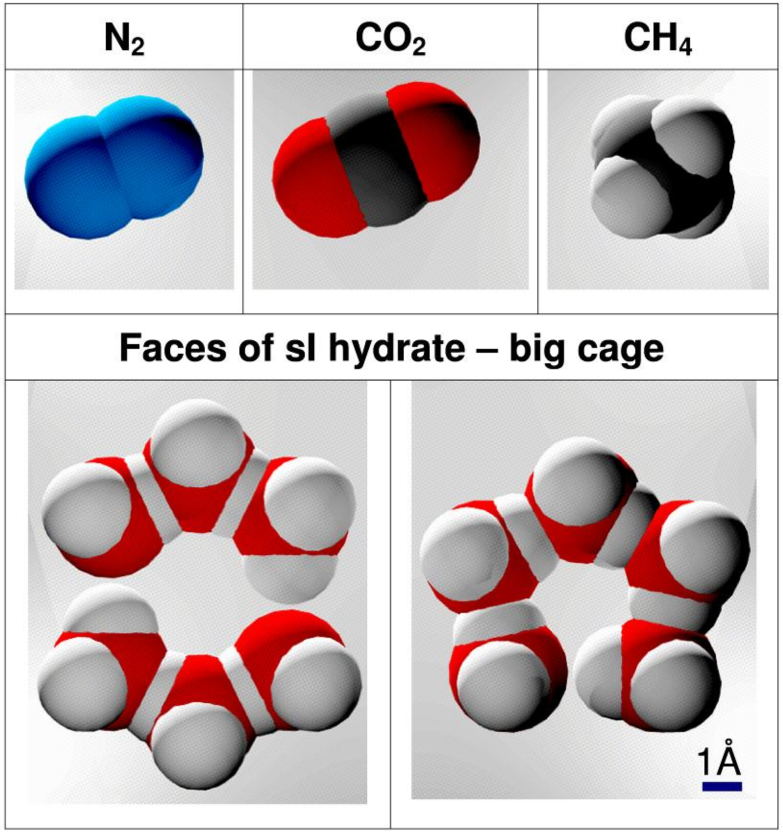
Carbon geological storage



Gas replacement in hydrates

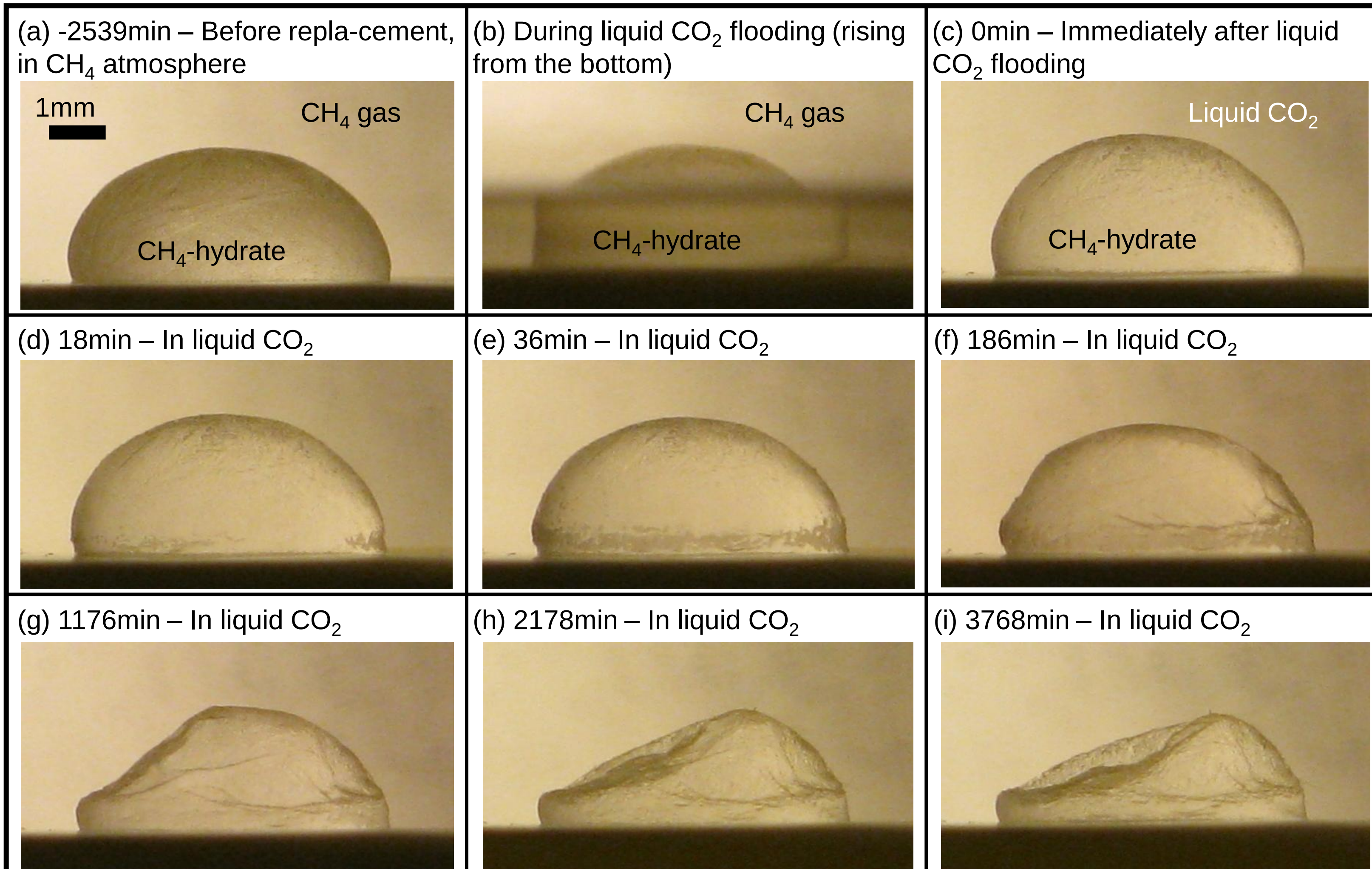


J Karl Johnson – NETL



Gas replacement in hydrates

CH_4 Hydrate flooded by liquid CO_2 P=6MPa, T=275K



(a) -2539min – Before repla-cement, in CH_4 atmosphere

(b) During liquid CO_2 flooding (rising from the bottom)

(c) 0min – Immediately after liquid CO_2 flooding

(d) 18min – In liquid CO_2

(e) 36min – In liquid CO_2

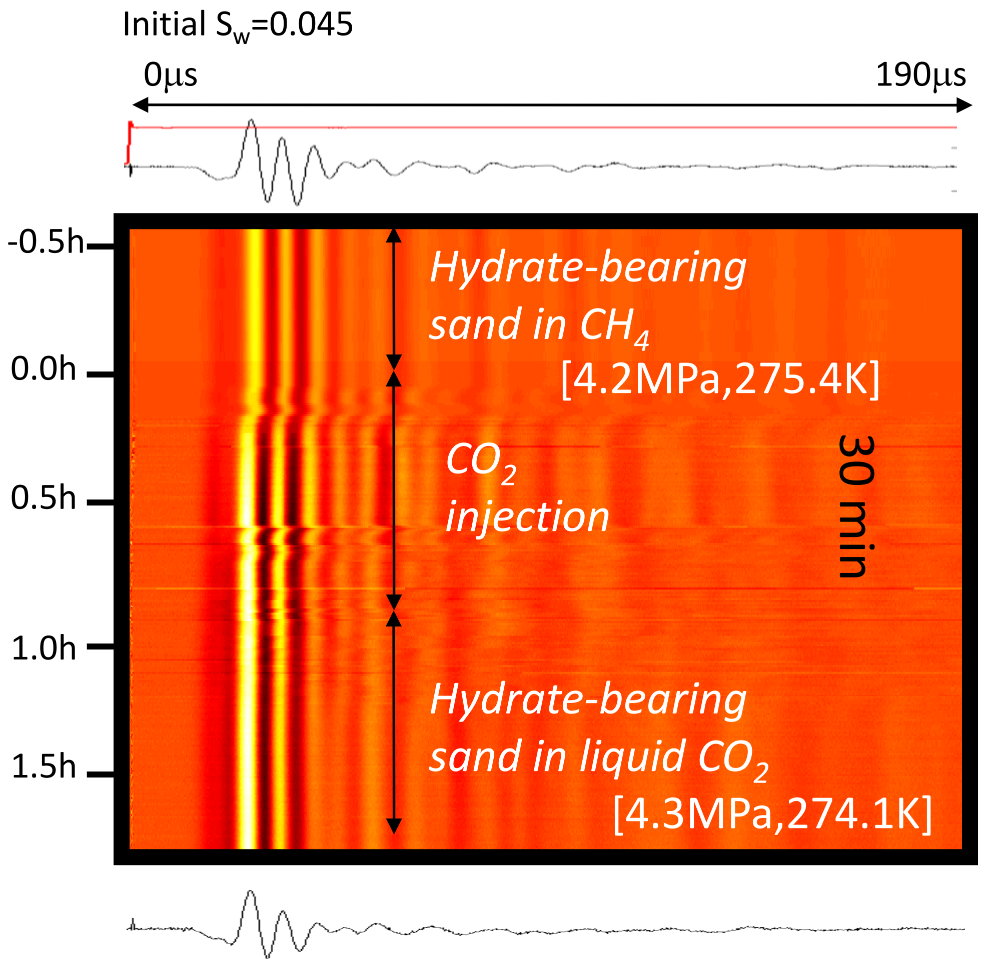
(f) 186min – In liquid CO_2

(g) 1176min – In liquid CO_2

(h) 2178min – In liquid CO_2

(i) 3768min – In liquid CO_2

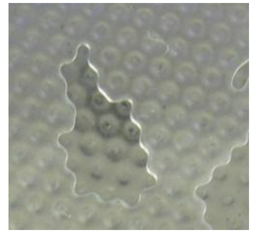
Gas replacement in hydrates



Summary

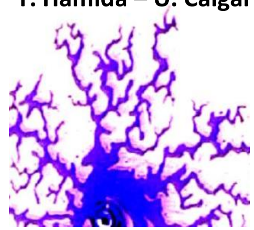
Carbon geological storage

Capillarity $C = \frac{v\ \mu_{CO2}}{\sigma \cos\theta}$



Viscosity $M = \frac{\mu_{CO2}}{\mu_{water}}$

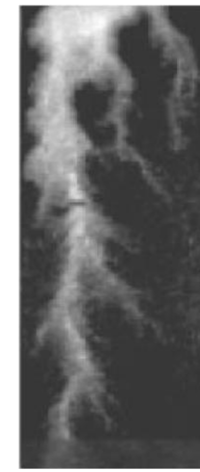
T. Hamida – U. Calgary



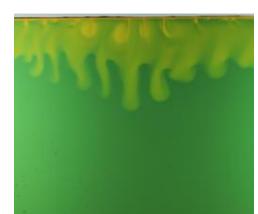
Buoyancy $B = \frac{(\gamma_w - \gamma_{CO2})\, k_w}{\sigma \cos\theta}$

Péclet $Pe = \frac{v\,\ell}{D}$

Damköhler $Da = \frac{\alpha\,\ell}{v}$



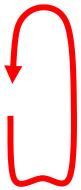
Convection /Advection $X = \frac{\mu\ v}{k\ \Delta\gamma}$



Summary: HCTM phenomena

Complex HTCM material properties and couplings

Potential development of positive feedback mechanisms



Caution: poor understanding of some "common" processes

New emergent phenomena in CO_2 geologic storage

Engineered injection

Sealing strategies (promote self-healing conditions)

CO_2-CH_4 replacement

Presentation Outline

Project Overview: ***The Proposal***

Accomplishments: **HTCM Coupled Processes**

Appendices: **Contact Information**

Schedule

Bibliography

Contact Information

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http://pmrl.ce.gatech.edu/

Project Schedule

Calendar Year	2010				2011				2012			
	Mar	Jun	Sept	Dec	Mar	Jun	Sept	Dec	Mar	Jun	Sept	Dec
Task #1 - Project Management and Planning	Team											
Task #2 - Experimental studies 2.1 Pore scale												Team
2.2 Dissolution												Team
2.3 Breakthrough / Self-heal												Team
Task #3 - Analyses – Scales – Parameter Domain												Team
Task #4 - Numerical Upscaling 4.1 Pore-scale phenomena												Team
4.2 Particle-scale phenomena												Team
Task #5 - Numerical Simulation: Coupled HCTM Processes												Team

Graduate Students (funded by this project)

PhD 1: D. N. Espinoza (Numerical)

PhD 2: S. Kim (Experimental)

Carlos Santamarina

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- Nicolas Espinoza (2011). CO2 sequestration – Fundamental Studies.

- Minsu Cha (2012). Mineral Dissolution - Implications.
- Jaewon Jang (2011). Gas Production from Methane Hydrates
- Jong Won Jung (2010). Gas Production from Methane Hydrates.
- Hosung Shin (2009). Discontinuities.

Journal Papers (6 additional papers in preparation – Contact PI)

- Espinoza, D.N. and Santamarina J.C., Clay interaction with liquid and supercritical CO2: The relevance of electrical and capillary forces, International Journal of Greenhouse Gas Control (submitted).
- Espinoza, D.N. and Santamarina J.C. (2010), Water-CO2-mineral systems: interfacial tension, contact angle and diffusion – Implications to CO2 geological storage, Water Resources Research, vol. 46, DOI: 10.1029/2009WR008634.
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- Shin, H., Santamarina, J.C. and Cartwright, J. (2010), Displacement Field In Contraction Driven Faults, J. Geophysical Research, 115, B07408, doi:10.1029/2009JB006572.
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- Jang, J., Narsilio, G. and Santamarina, J.C. (2011), Hydraulic Conductivity in Spatially Varying Media -A Pore-Scale Investigation, Geophysical Journal International, vol. 184, pp. 1167-1179