DOE-ARRA Geologic Sequestration
Training and Research
2011 Yearly Review Meeting

CO_2 Geological Storage: Coupled THCM Phenomena

(*from pore-scale to macroscale implications)*

PI: J. Carlos Santamarina

Georgia Institute of Technology
School of Civil and Environmental Engineering
February 24-26, 2011

Introduction: "*a Faustian bargain*"?

Context: Geological storage of CO_2

- Necessary a worldwide C-economy facing climate change
- Must be reliable in short-and-long time scales

Main concerns:

- Complex, coupled hydro-chemo-thermo-mechanical processes
- Unrecognized emergent phenomena
- Positive feedback mechanisms, runaway effects
- High early probability of failure
- Exergy drop in leaky systems
- Engineered self-healing systems?

Without paralyzing the critically needed development of CCS strategies:

- Anticipate potential challenges while still at the laboratory/model scale
- Develop proper engineering solutions

Project Objectives

better understanding of fundamental processes and couplings that may either hinder or enhance the long-term geological storage of CO_2.

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**

Our approach will combine:

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

Project Participants

J. Carlos Santamarina
Principal Investigator

N Espinoza

SH Kim

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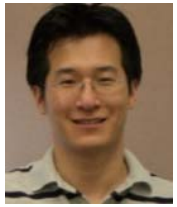
N Espinoza

J.W. Jung
CO_2-CH_4

SH Kim



J. Jang
Networks

M.S. Cha
Dissolution

H.S. Shin
Dissolution

L.Velasco
U Andes
Modeling

ES Bang
KIGAM
Monitoring

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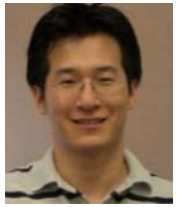

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Collaborators (no cost)

G. Goldsztein	***GT-Math***	***Analyses***
M. Sanchez	***Texas A&M***	***FEM Modeling***
M. Dusseault	***U. Waterloo***	***Field phenomena***
A. Lizcano	***U. Andes***	***Modeling***

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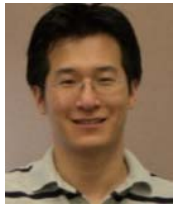

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Chemo-physical Coupling
water-CO_2 interaction
fluid-mineral Interaction
contact angle & surface ten.

CM Coupling: Caprock
clay-CO_2
slab effect

HCM Coupling
reactive transport
mineral dissolution
fluid-driven fracture

TCM Coupling
CO_2-CH_4 replacement

Modeling

Monitoring

Healing

Highlights of Project - Accomplishments

- **Phenomena**
  - contact angle and surface tension = f(P,T)
  - effective stress field during dissolution
  - CO_2-CH_4 replacement

- **Analytical**
  - caprock response following dissolution

- **Experimental**
  - high-pressure cells for pore-scale studies
  - high-pressure cells for caprock studies
  - cells for CO_2 leak visualization

- **Numerical**
  - network model for reactive fluid transport

Project Funding

- **Total Project Cost:** **$300,000**
- **DOE Share:** **$300,000**
- **Non-DOE Cost Share:** **n/a**

- **Collaborations (no cost):** **Texas A&M**
  Industry (USA)
  U. Waterloo (Canada)
  U. Andes (Colombia)

Tasks – Overview

Task No.	Task Description	Task Duration	Task Funding
1.0	Project Management	1/2010 – 12/2012	3,772 .
2.0	Experimental Studies	1/2010 – 12/2012	137,117 .
3.0	Analysis - Scales - Parameter Domain	1/2010 – 10/2011	17,463 .
4.0	Numerical Upscaling	6/2010 – 12/2011	130,322 .
5.0	Numerical Simulation - HTCM	6/2010 – 12/2012	*collaboration*

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)

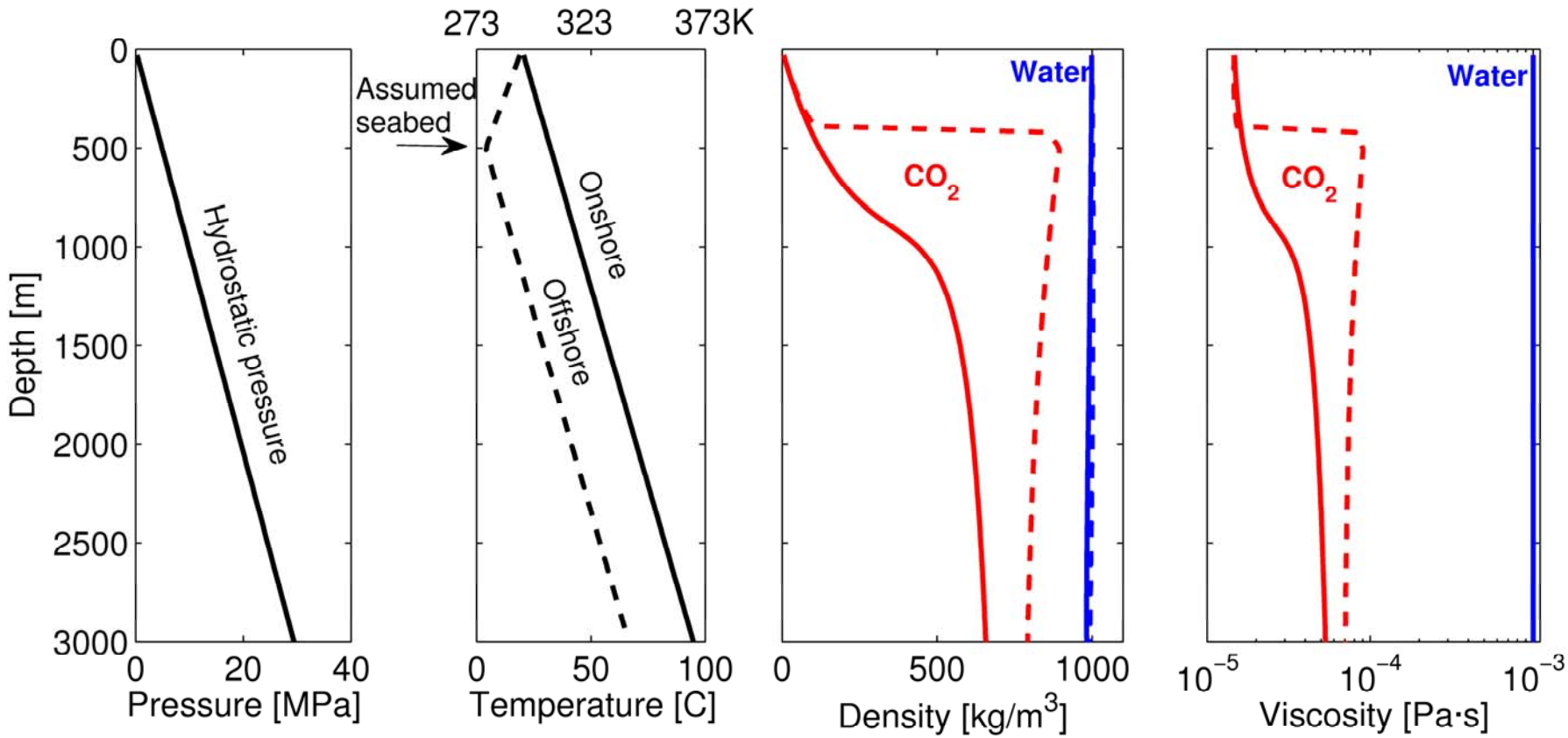
- PhD 1: D. N. Espinoza (Numerical)
- PhD 2: S. Kim (Experimental)
- Carlos Santamarina

T2: 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

Participants:	Status:	Accomplishments:	Issues:
Espinoza & Kim	**90%**	**comprehensive**	**kinetics**

T2: Physical Properties



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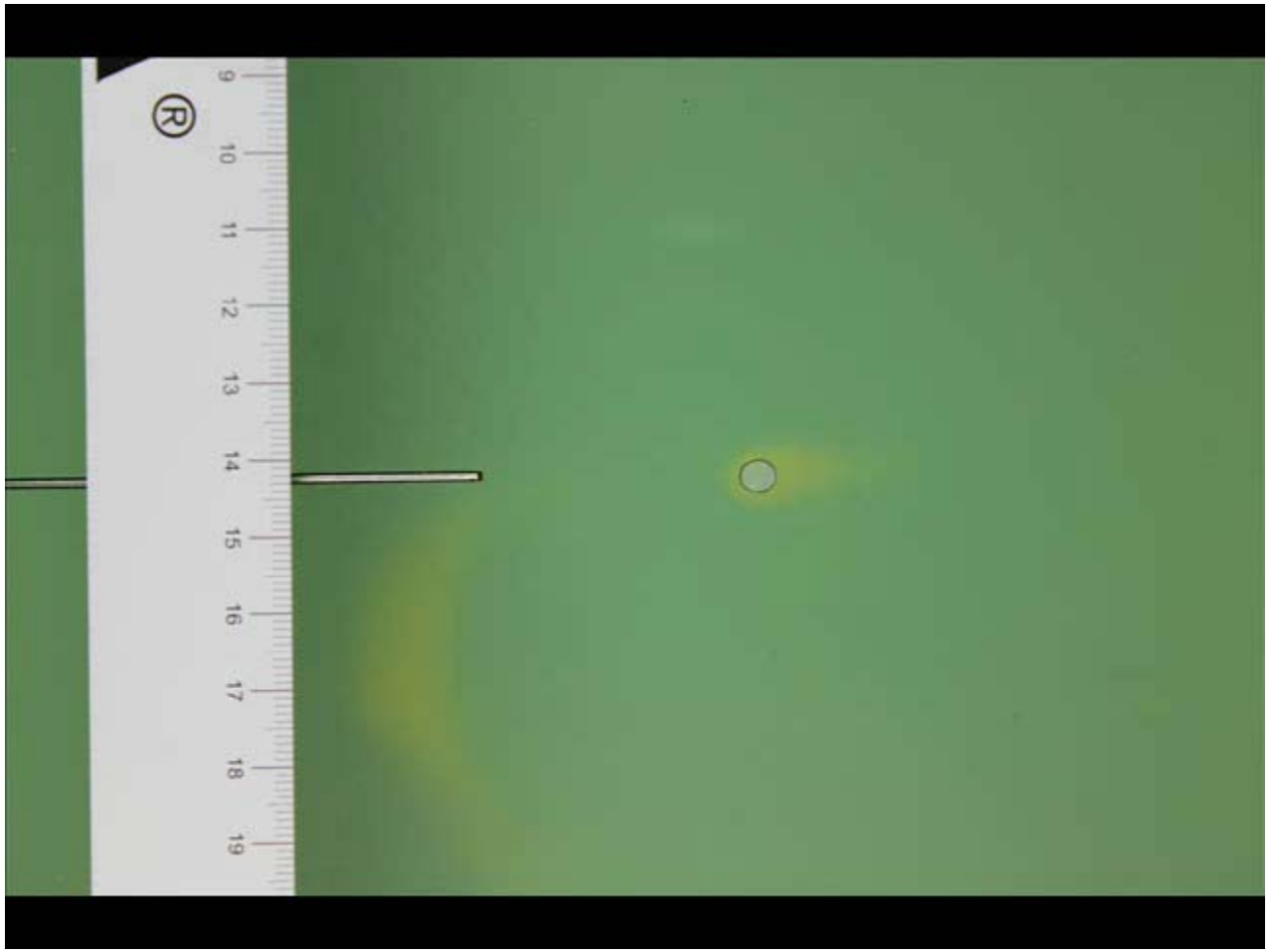
T2: H_2O+CO_2: Acidification



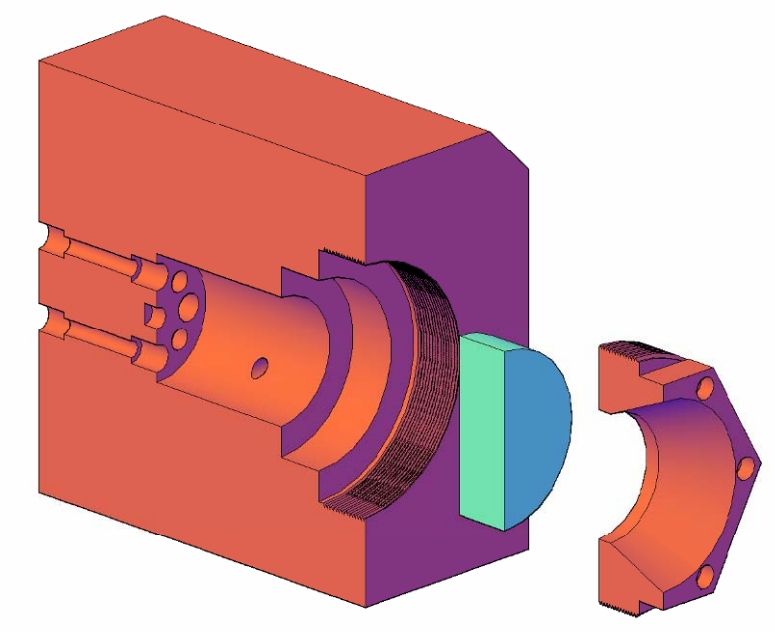
Participants:	Status:	Accomplishments:	Issues:
Bang	40%	visualization	high pressure

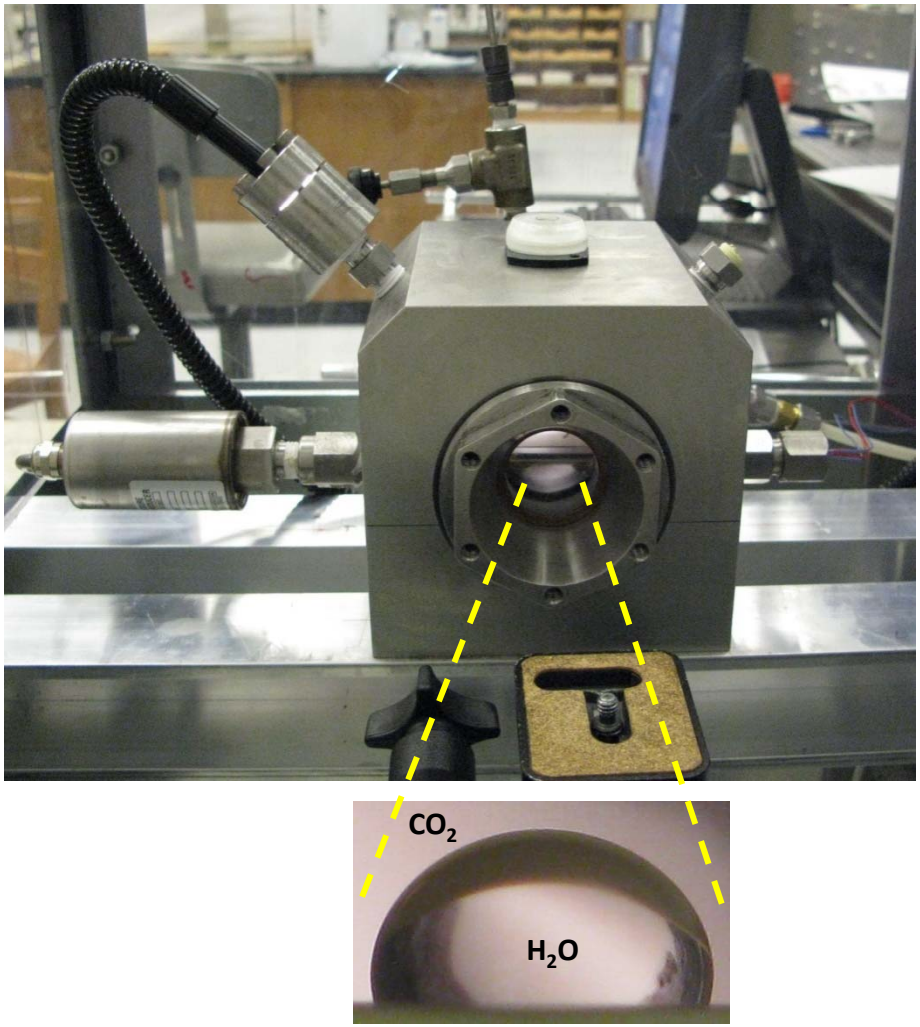
T2: H_2O+CO_2: Acidification – Monitoring?

480 x speed (6.5hours)

Participants:	Status:	Accomplishments:	Issues:
Bang	40%	visualization	high pressure

T2: Surface Tension and Contact Angle





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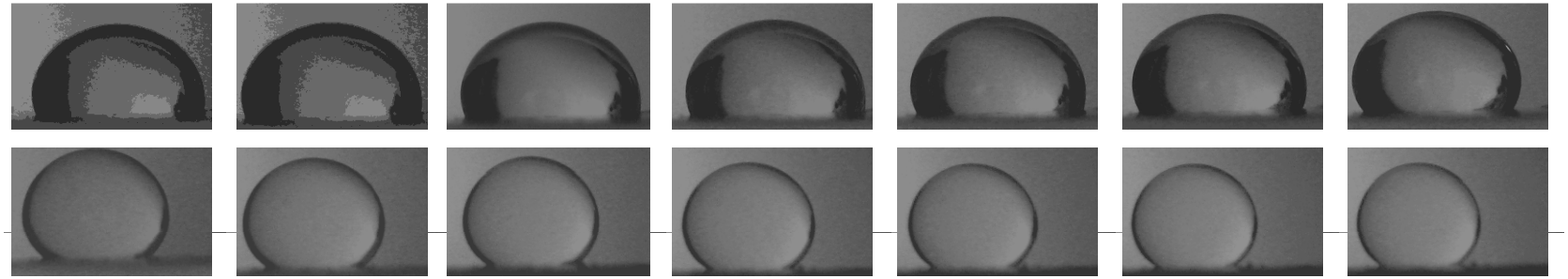
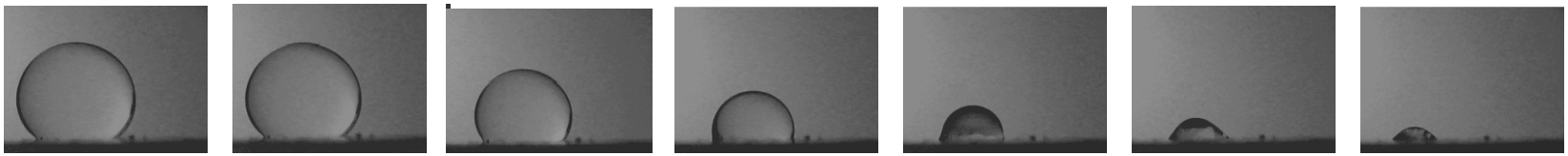
T2: Surface Tension and Contact Angle

Increasing CO_2 pressure: changes in contact angle and surface tension



Hold Test in Liquid CO_2: Water diffusion



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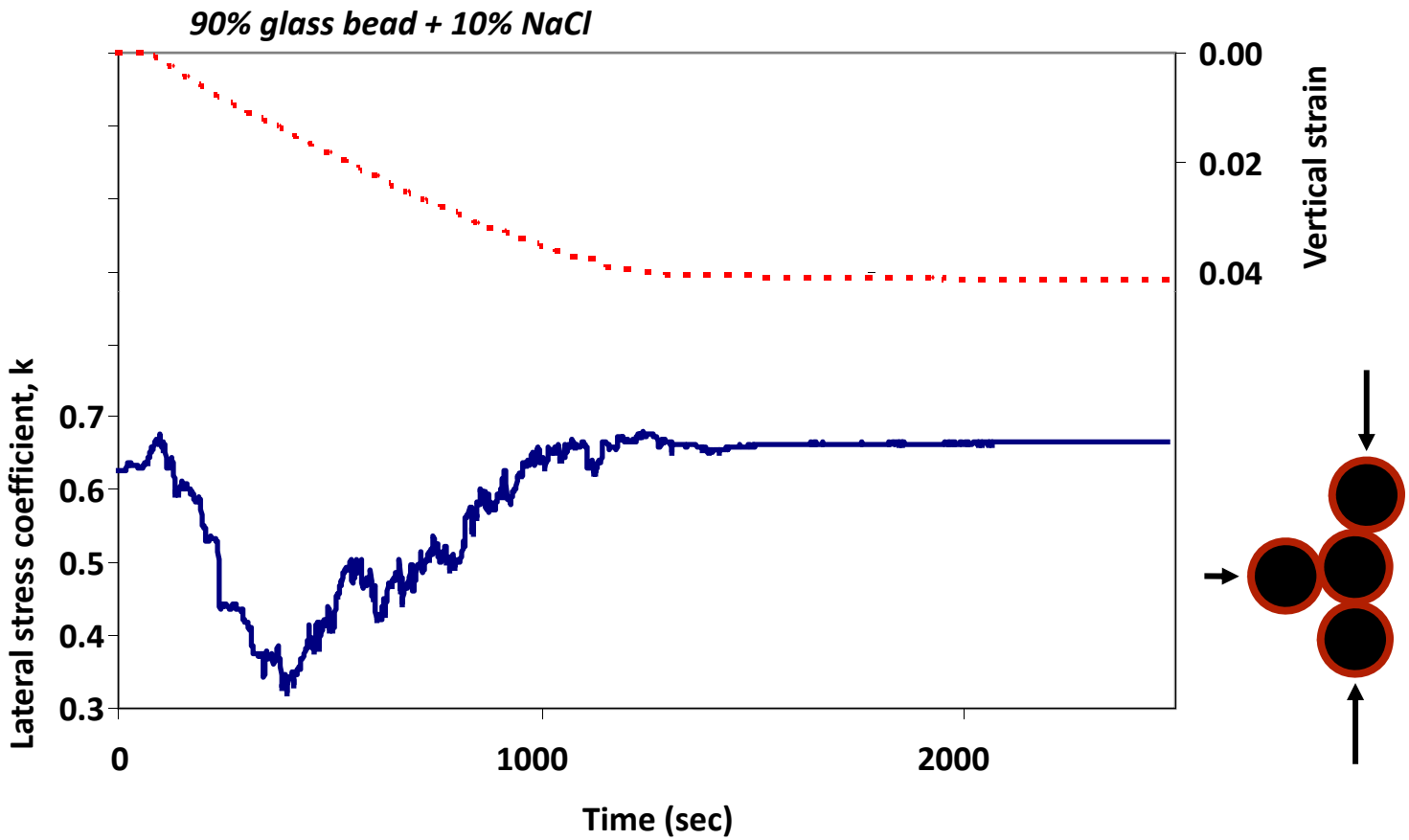
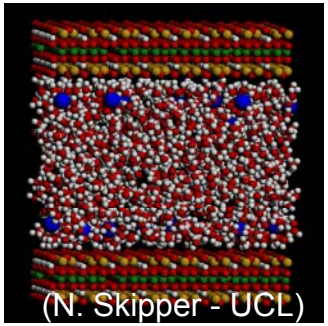
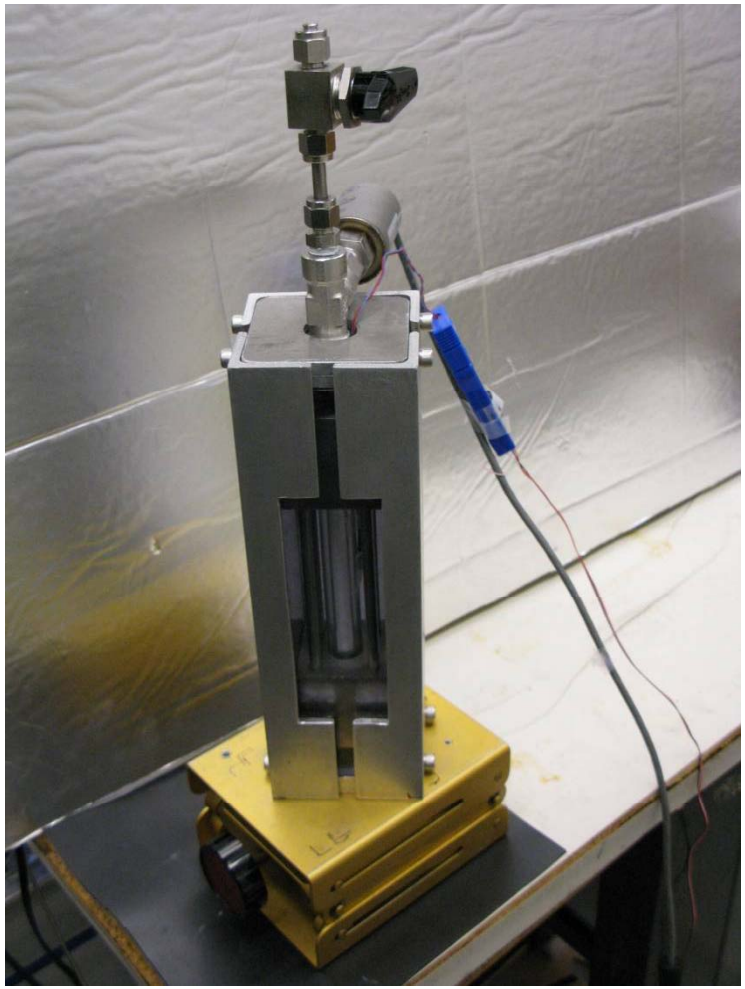
T2: Mineral Dissolution - Implications



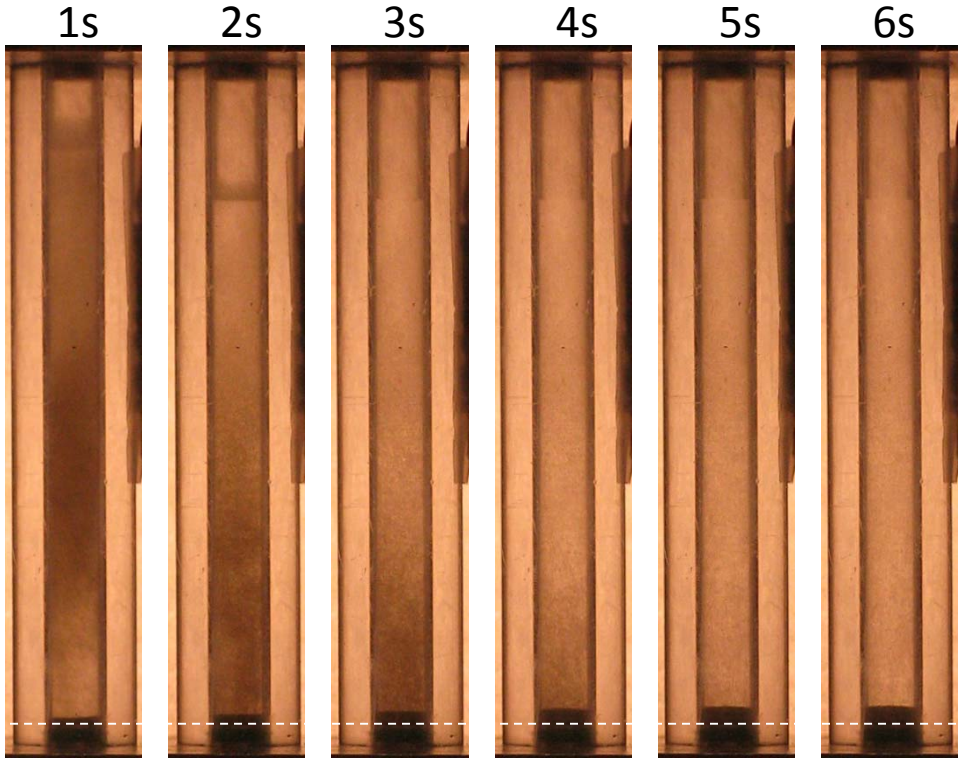
Participants:	Status:	Accomplishments:	Issues:
Shin & Cha	80%	comprehensive	extension to CO_2

T2: Clay-CO_2 interaction





montmorillonite in liquid CO_2



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Espinoza	60%	pore fluid effects	DLVO analysis

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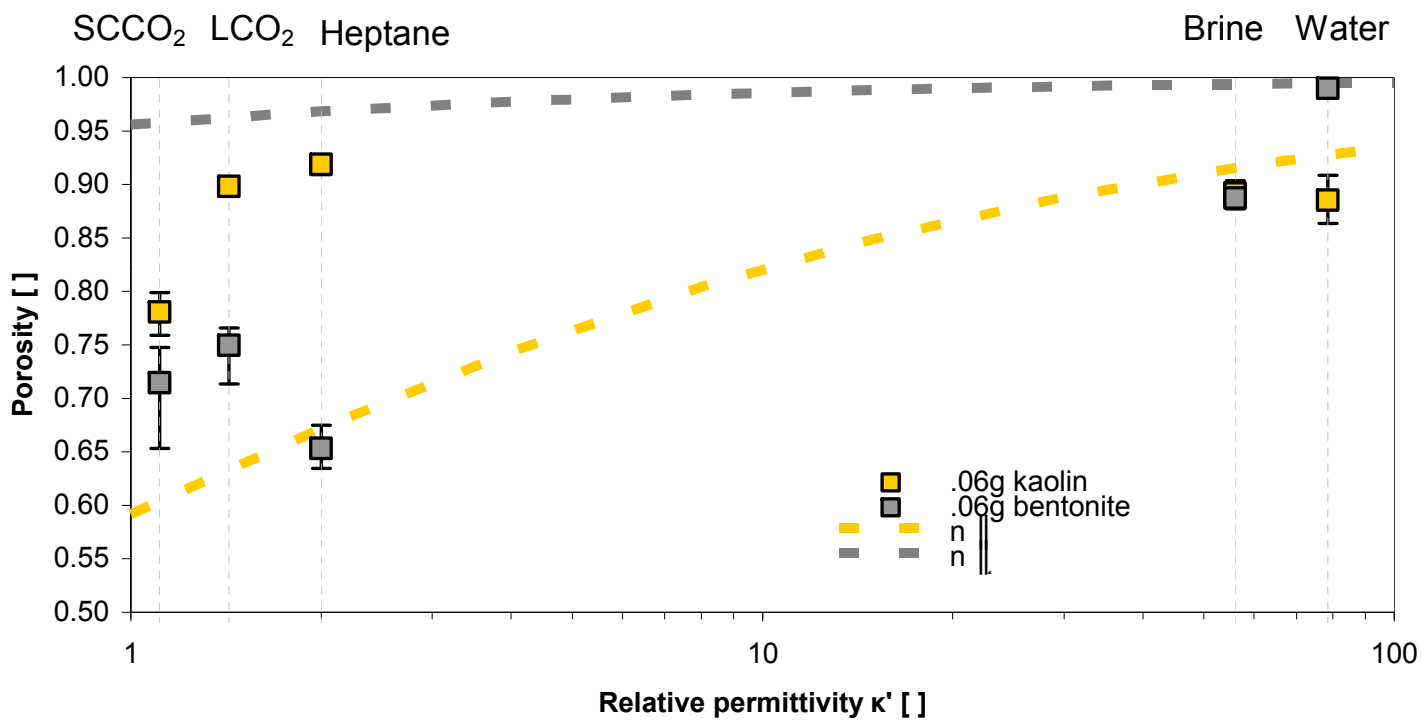

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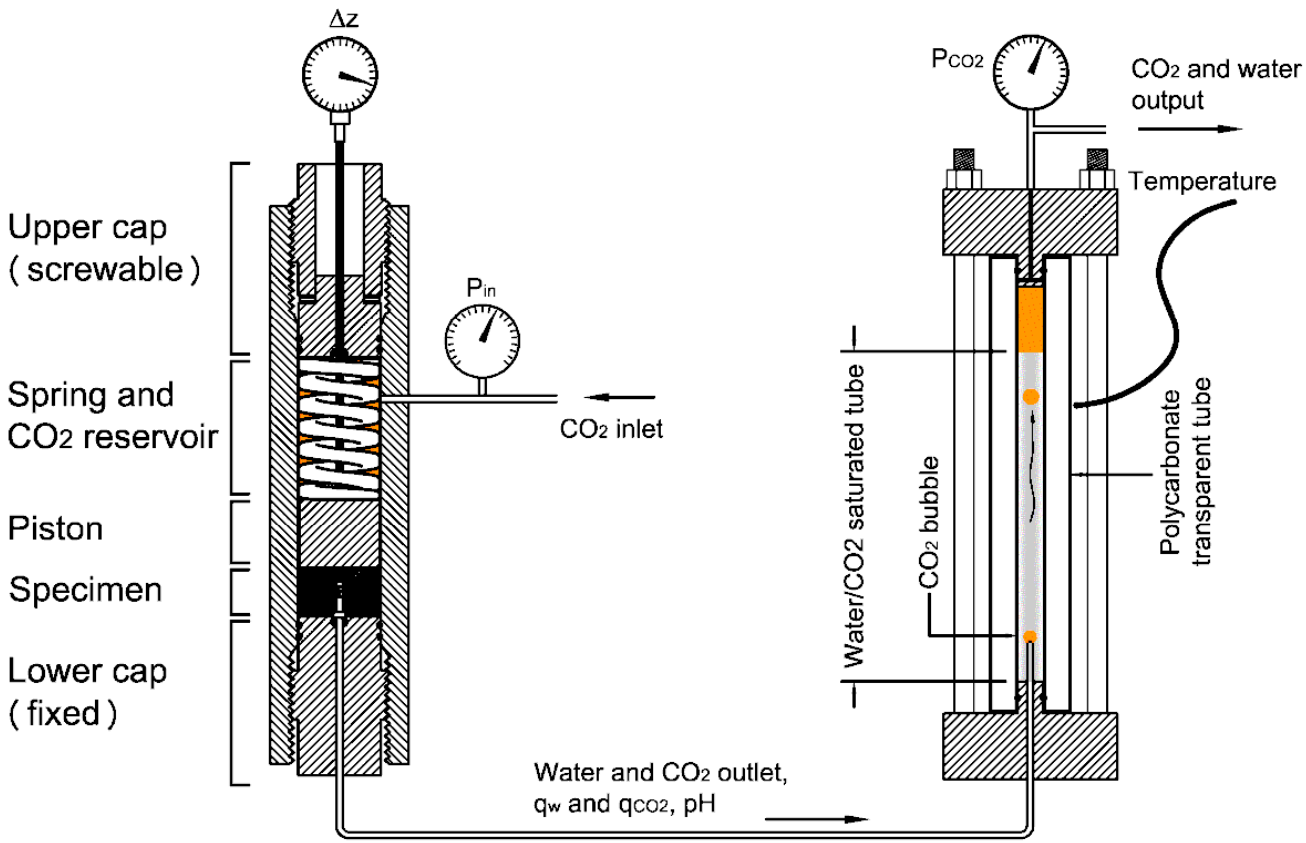
T2: Breakthrough - Healing



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Espinoza	40%	device and prelim results	causal link

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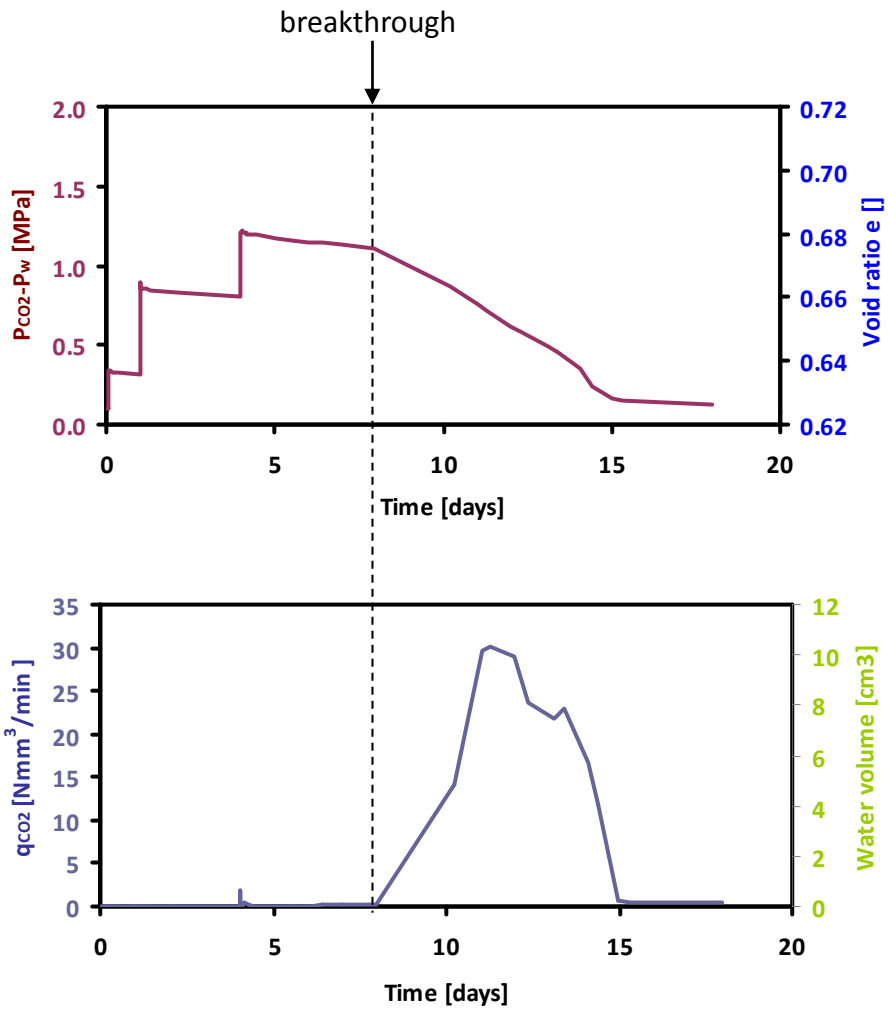

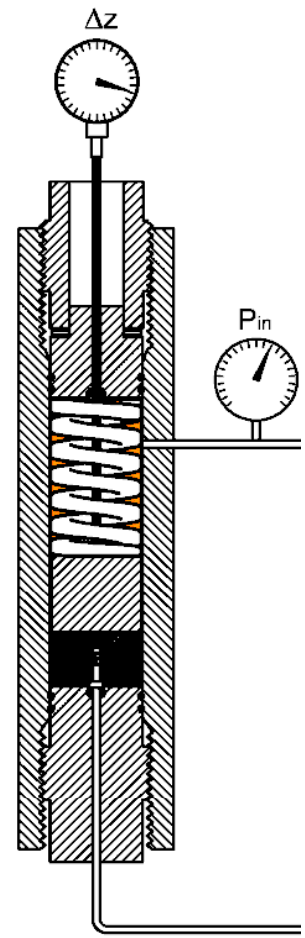

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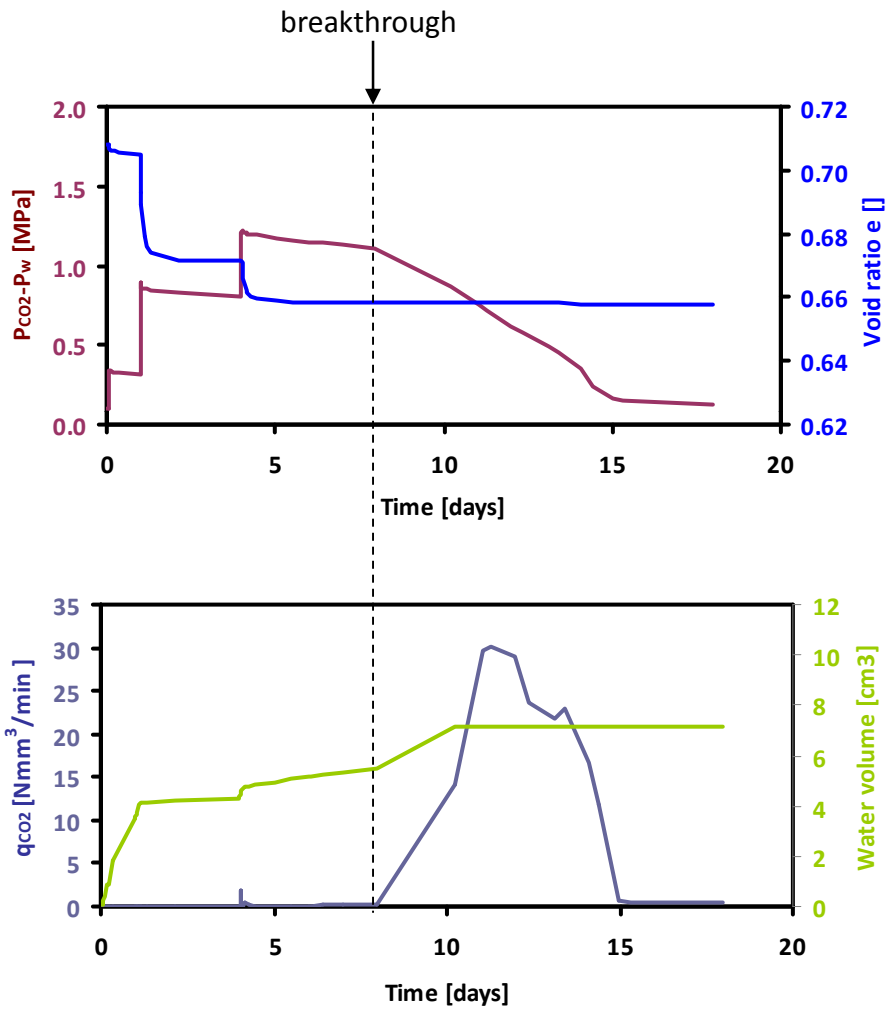

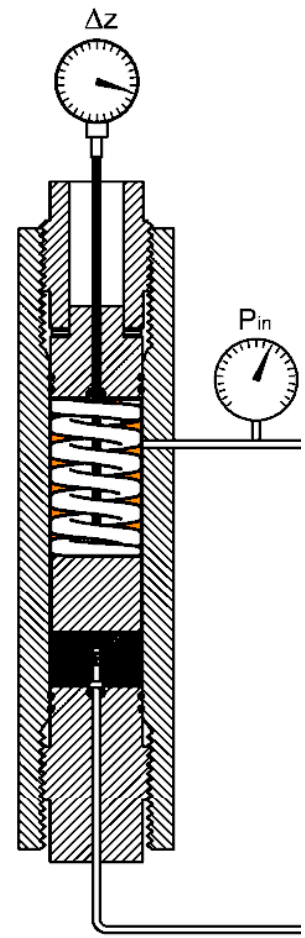

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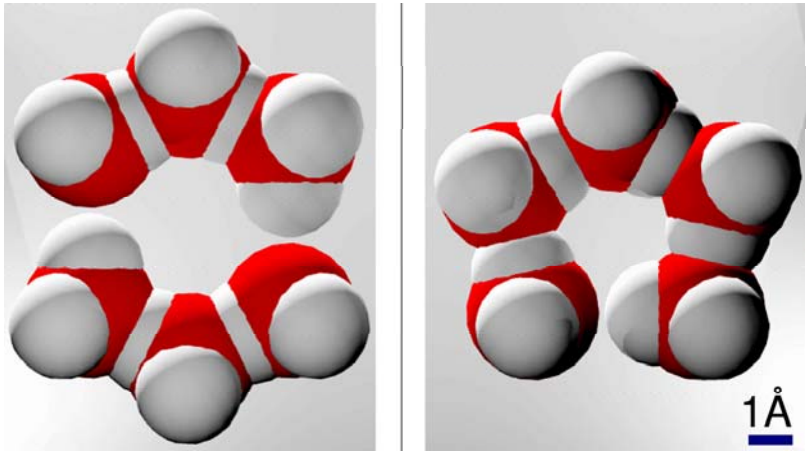
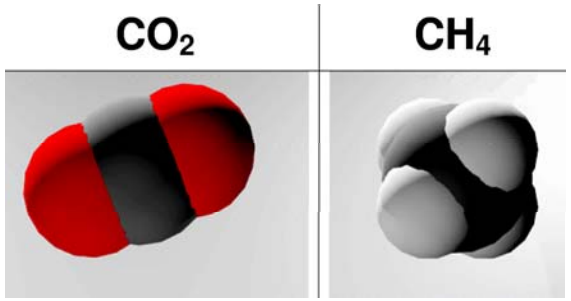
Espinoza	40%	device and prelim results	causal link

T2: Hydrates: CO_2-CH_4 Replacement





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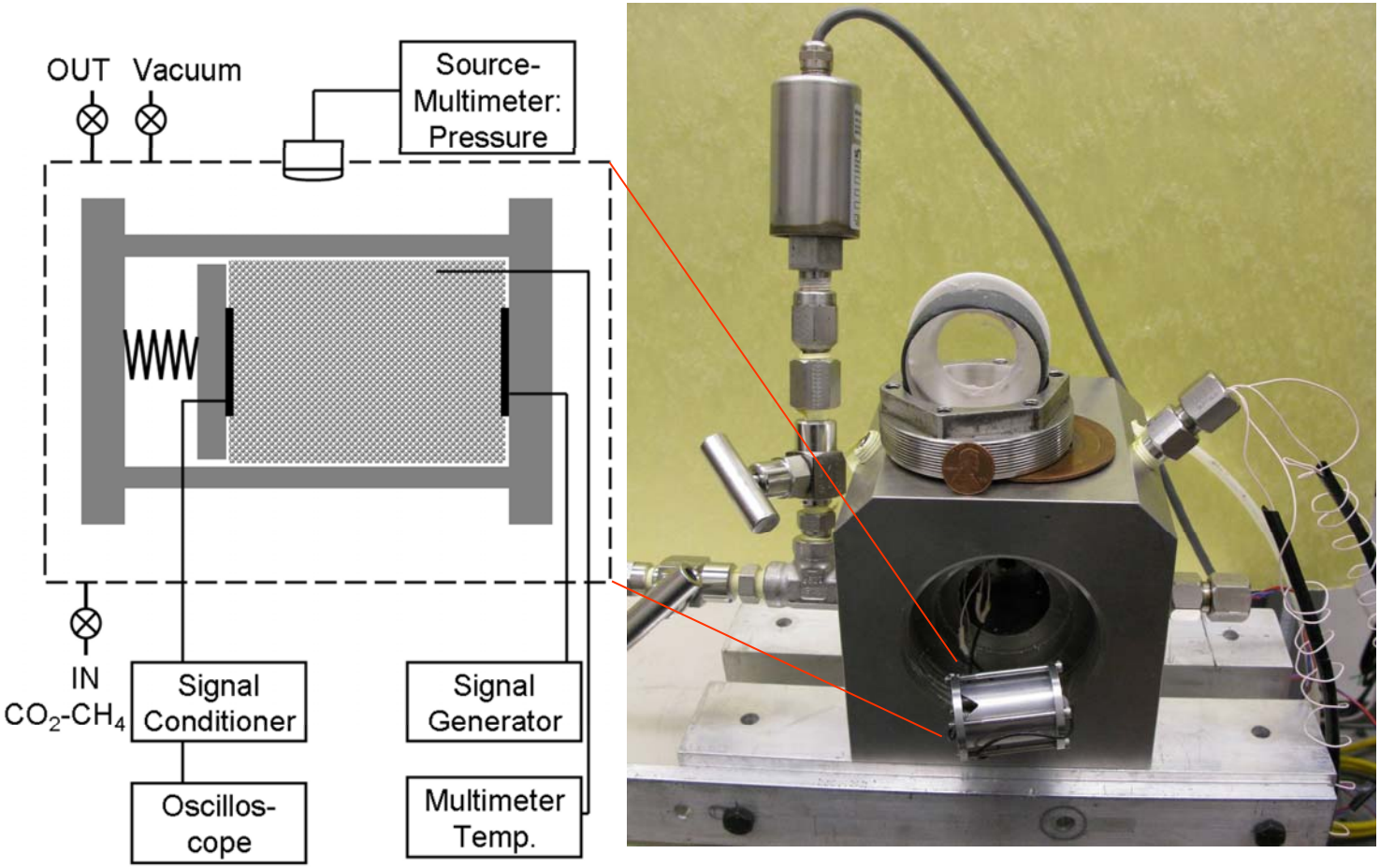

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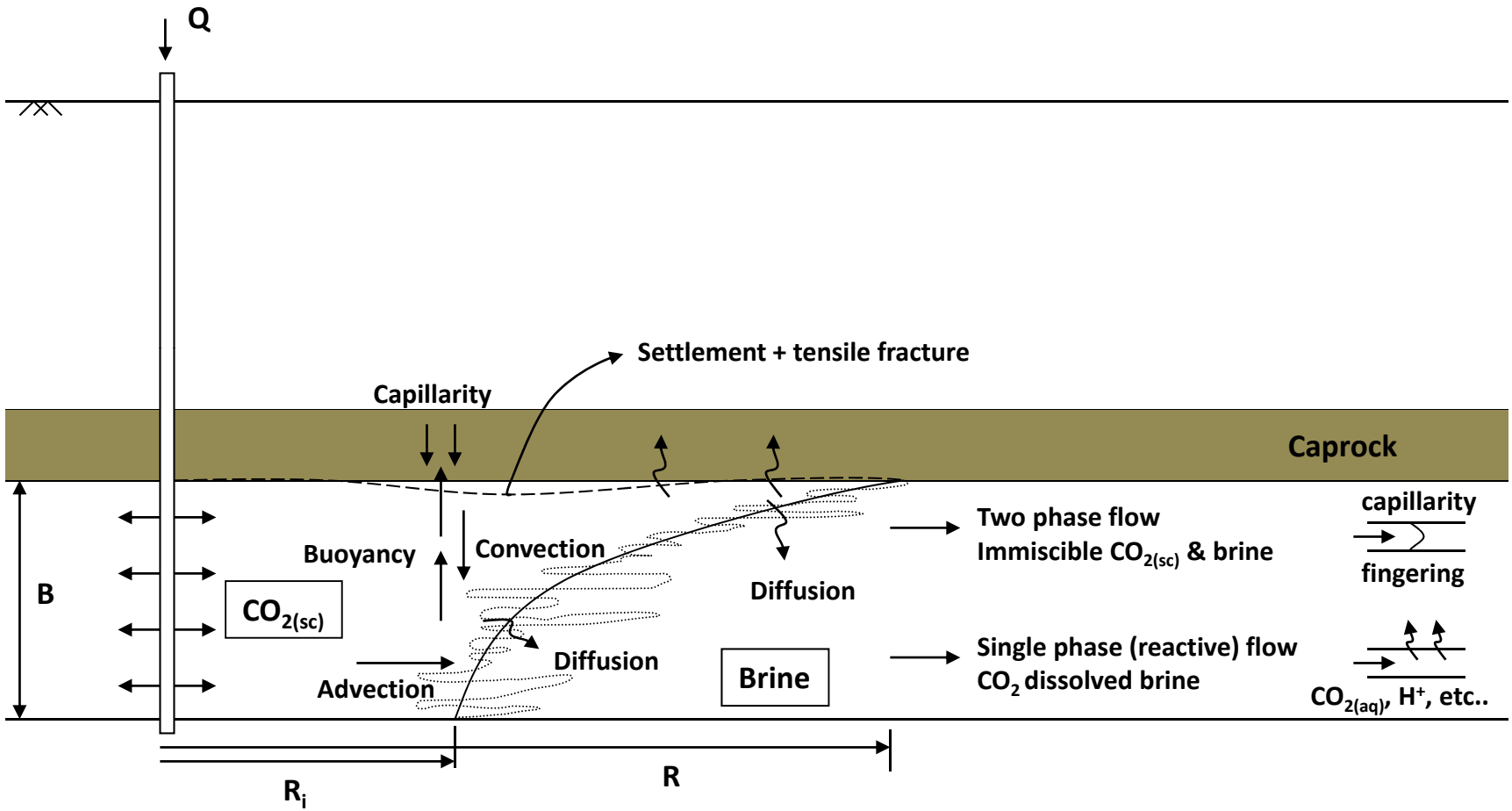
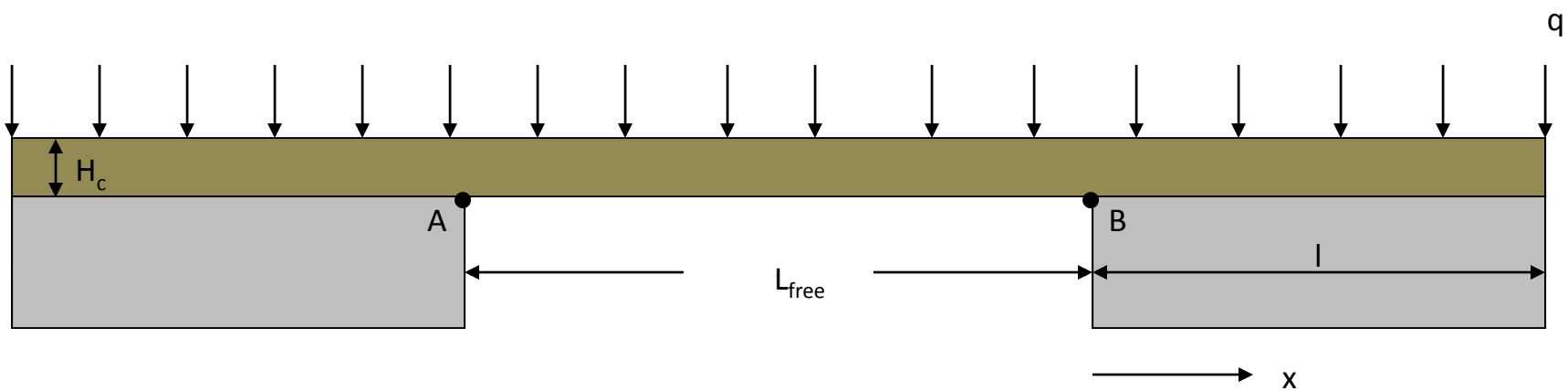
T3: Analyses – Parameter range



Participants:	Status:	Accomplishments:	Issues:
Kim	50%	key π-ratios	parameter regime

T3: Analyses – Parameter range

$$\lambda = \sqrt[4]{\frac{k_r}{4E_c I_c}}$$



$$\pi_1 = \frac{\rho_c g z_c}{\sigma_y} \qquad \pi_2 = \frac{L_{free}}{H_c} \qquad \pi_3 = \lambda H_c \qquad \pi_4 = \frac{\sigma_{t\max}}{\sigma_y}$$

Participants:	Status:	Accomplishments:	Issues:
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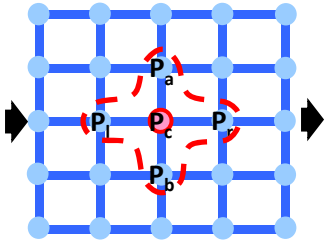
T4: Upscaling – Network Models



Initial conditions: pH = 8.26

→ $[H^+]_0 = 5.5\times10^{-9}$ mol/l

$[CO_{2(aq)}]_0 = 1.1\times10^{-5}$ mol/l

$[HCO_3^-]_0 = 8.96\times10^{-4}$ mol/l

$[Ca^{2+}]_0 = 4.34\times10^{-4}$ mol/l

$c_{i,j}(0) = c_0,\ j > 1$

Inlet pressure = P_{in}

CO_2 dissolved water

pH = 3.28

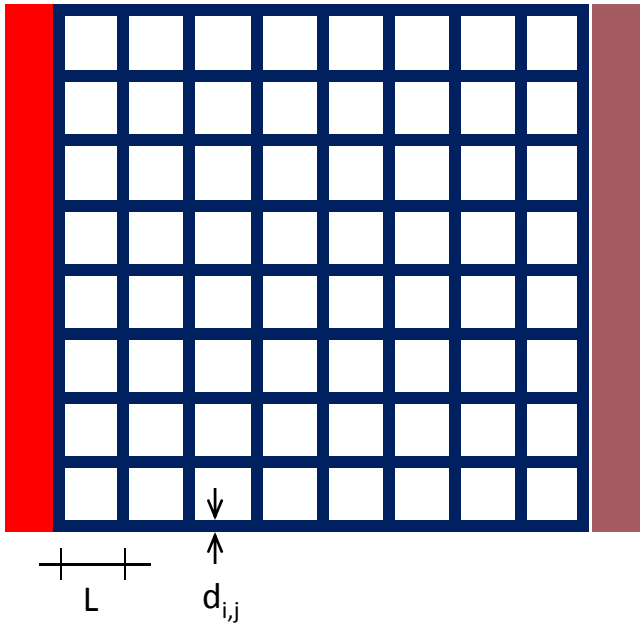
→ $[H^+] = 10^{-3.28}$ mol/l

$[CO_{2(aq)}] = 1.66$ mol/l

$[HCO_3^-] = 0.0014$ mol/l

$[Ca^{2+}] = 4.34\times10^{-4}$ mol/l

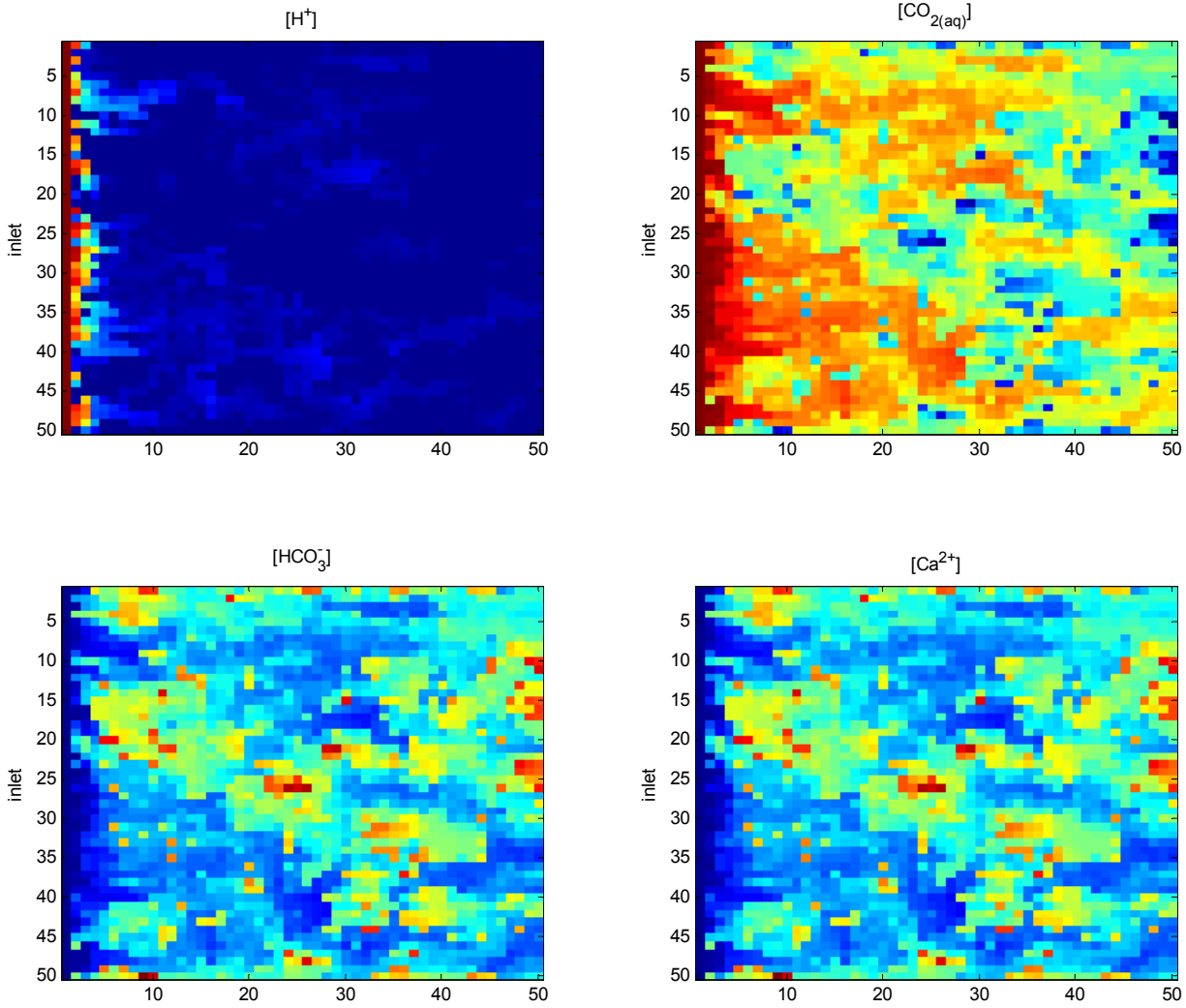
$c_{i,1}(t) = c_{inlet}$



Outlet pressure = P_{out}

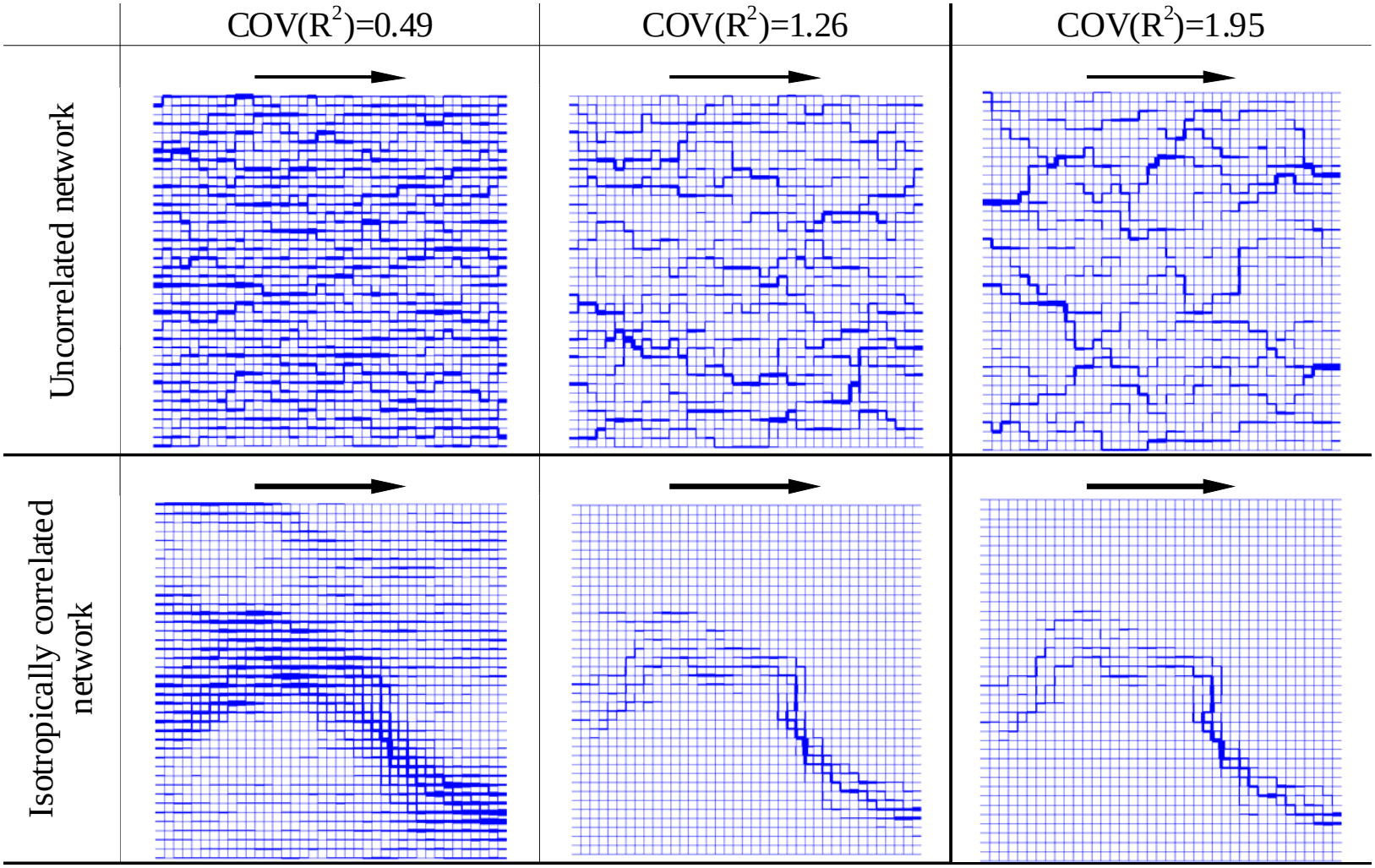
Participants:	Status:	Accomplishments:	Issues:
Kim	50%	robust & versatile algorithm	input parameters

T4: Upscaling – Network Models



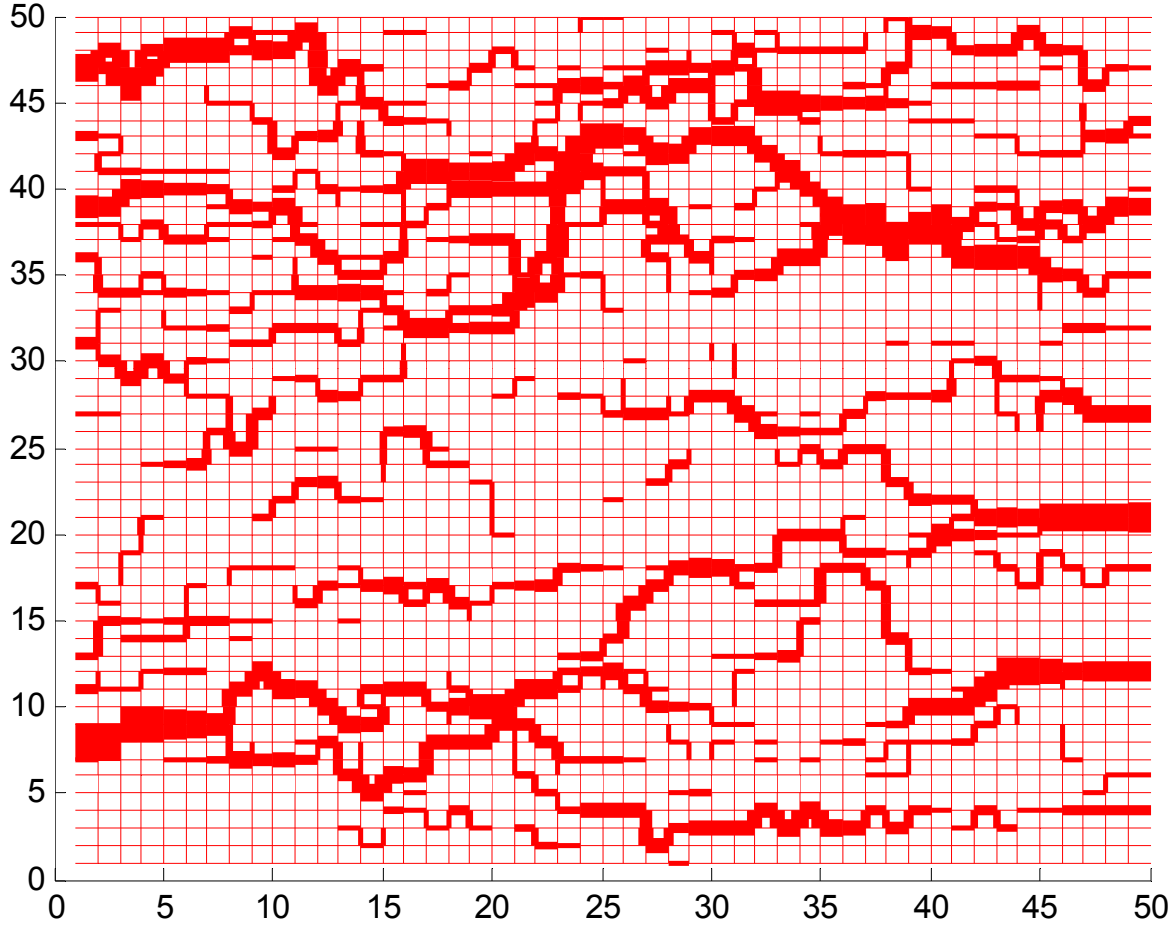
Participants:	Status:	Accomplishments:	Issues:
Kim	50%	robust & versatile algorithm	input parameters

T4: Upscaling – Non-Reactive



Participants:	Status:	Accomplishments:	Issues:
Kim (& Jang)	50%	robust & versatile algorithm	input parameters

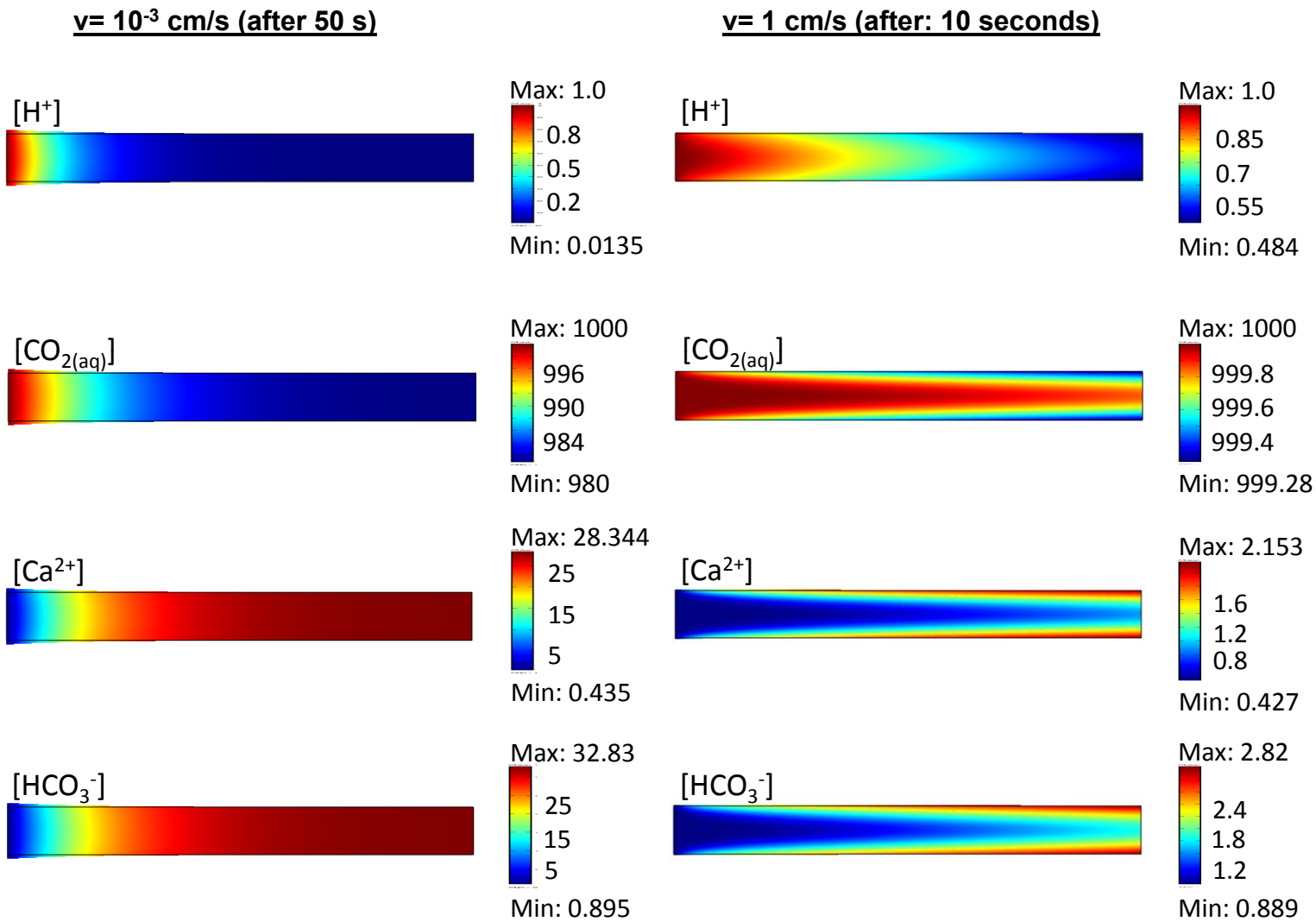
T4: Upscaling – Reactive



Participants:	Status:	Accomplishments:	Issues:
Kim (& Jang)	50%	robust & versatile algorithm	input parameters

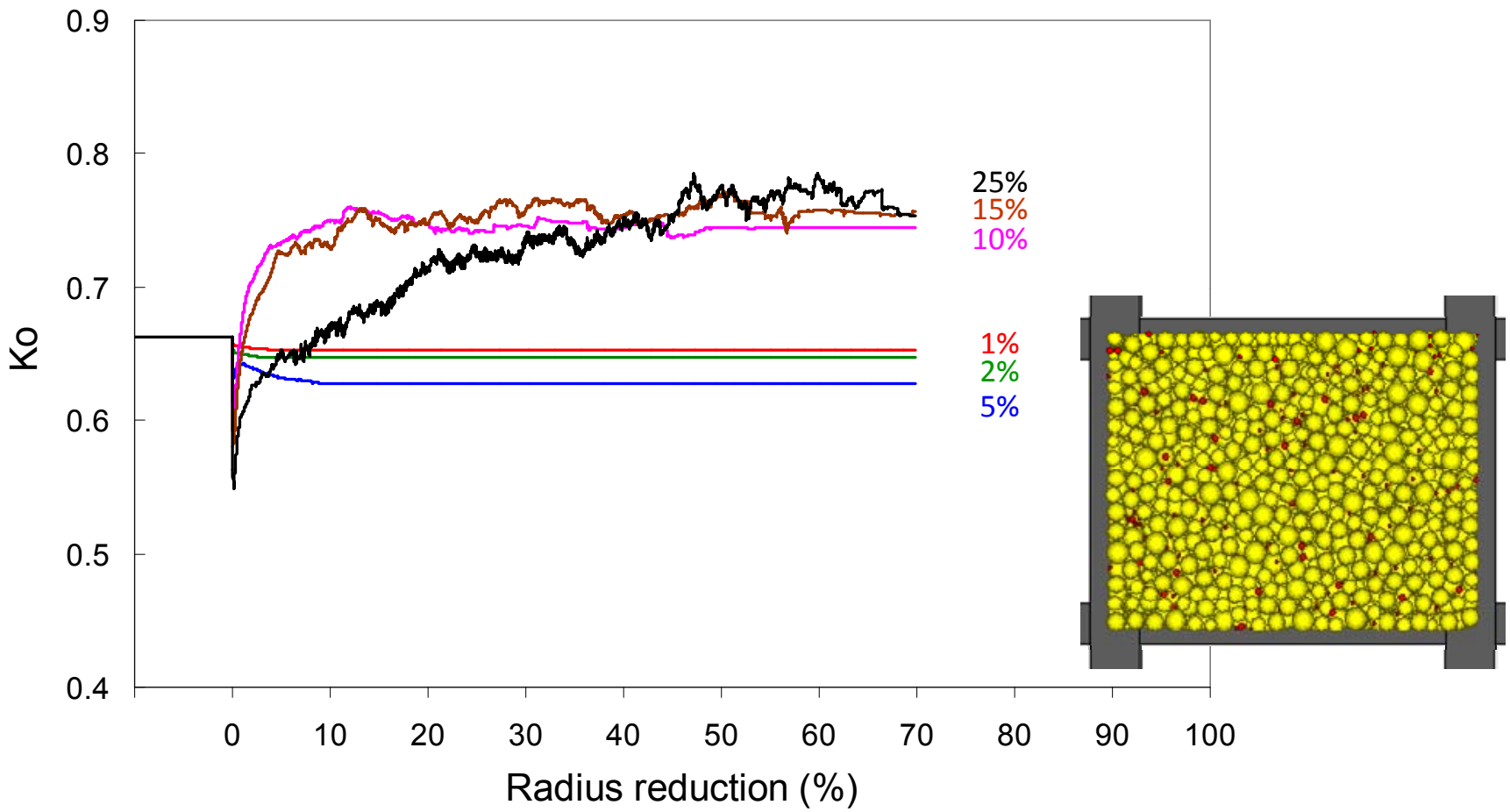
T4: Reactive Fluid Flow - Fractures

calcite dissolution
fracture aperture 10 [μm]
fracture length 100 [μm]



Participants:	Status:	Accomplishments:	Issues:
Kim	30%	validation	computational demand

T4: Upscaling Particle Dissolution



Participants:	Status:	Accomplishments:	Issues:
Shin & Cha	90%	experimental & numerical	CO_2 extension

Project Tasks and Milestones

TASKS	Target	Completed
complete construction of new surface&2D net studies (Task 2.1)	03/31/10	03/19/10
identification and compilation of governing parameters (Task 3)		03/31/10
preliminary tests on surface effects (Task 2.1)	06/30/10	01/30/10
development of analytical models (Task 3)		06/30/10
complete pore scale studies (Task 2.1)	09/30/10	09/30/10
completion of analytical formulation (task 3)		09/30/10
complete construction of enhanced oedometric cell (Task 2.2)	12/31/10	12/31/10
evaluate different scenarios using analytical models and their implications (Task 3)		12/31/10
preliminary tests on dissolution effects (Task 2.2)	03/31/11	
preliminary upscaling model results using network models (Task 4.1)		
complete experimental studies on dissolution effects (task 2.2)	06/30/11	
completion of upscaling model results using network models (Task 4.1)		
adaptation oedometric cell for breakthrough studies (Task 2.3)	09/30/11	
preliminary upscaling model results using DEM models (Task 4.2)		
preliminary results on breakthrough (Task 2.3)	12/31/11	04/10/10
completion of upscaling model results using DEM models (Task 4.2)		
complete experimental studies on breakthrough (Task 2.3)	03/31/12	
FEM code adaptation for fully coupled formulation (Task 5)		
extend breakthrough studies to explore self-healing conditions (Task 2.3)	06/30/12	
preliminary results with FEM code (Task 5)		
complete self-healing study (Task 2.3)	09/30/12	
complete study using FEM code (Task 5)		
PROJECT COMPLETION	12/31/12	

Anticipated Efforts for the Coming Year

- Advance all tasks (experiments, analyses, simulations)
- Workshop (*with deliverable*)
- Submit key results for publication
- Update "Energy Geotechnology" course
- Graduation: 1 PhD (Espinoza)
- Admission: 1 New PhD

PI Contact Information

Questions, collaboration, scientific visit/stay?

Please contact:

J. Carlos Santamarina
404-894-7605
jcs@gatech.edu

Workshop: to be announced … !