Monitoring of Geological CO_2 Sequestration Using Isotopes & PFTs

Project Number FEAA-045

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U.S. Department of Energy

National Energy Technology Laboratory

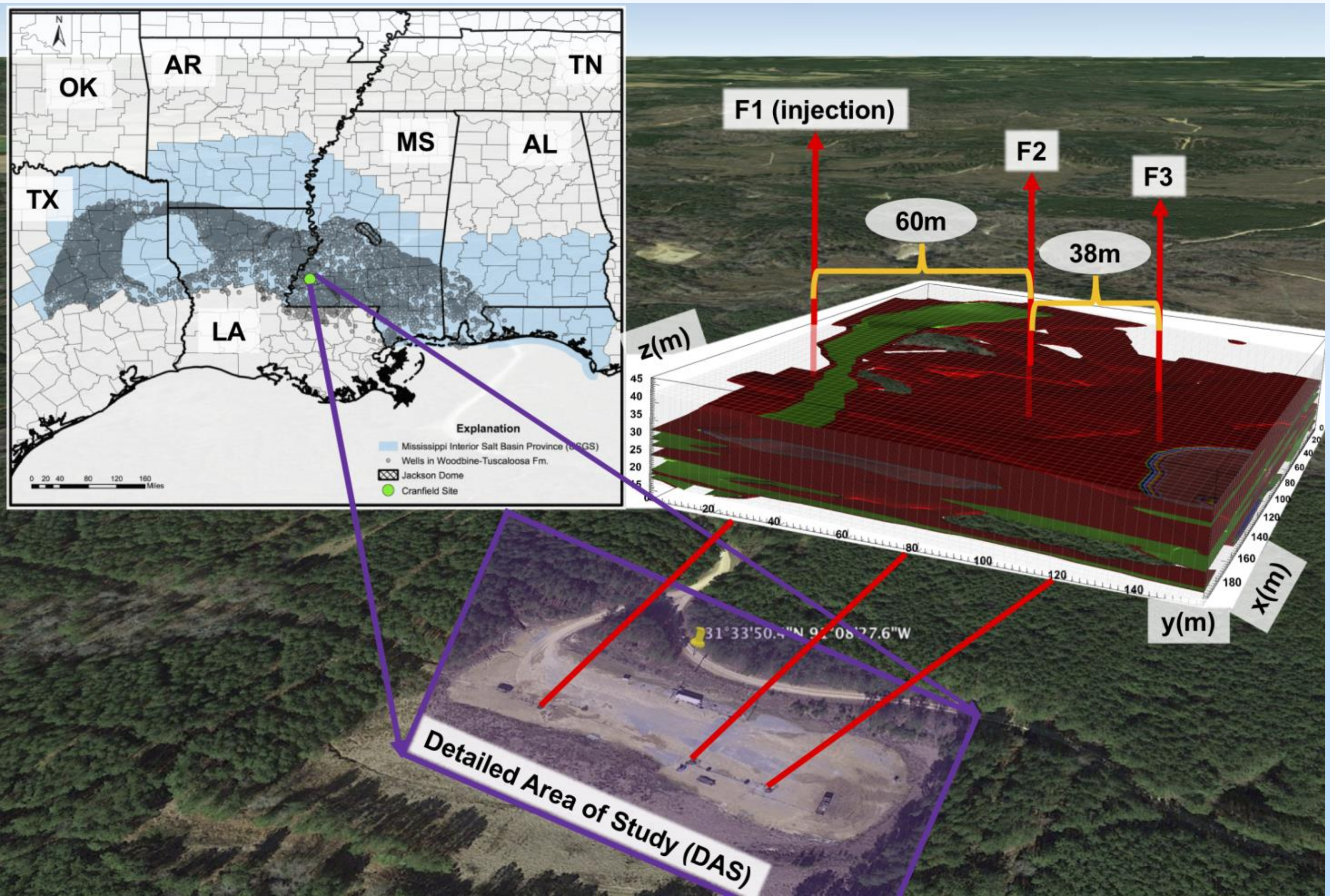
Carbon Storage Project Review Meeting

2021 Virtual Review Webinar

August 9, 2021

Project Overview

Provide methods to interrogate the subsurface that will allow direct improvement of CO_2 storage.



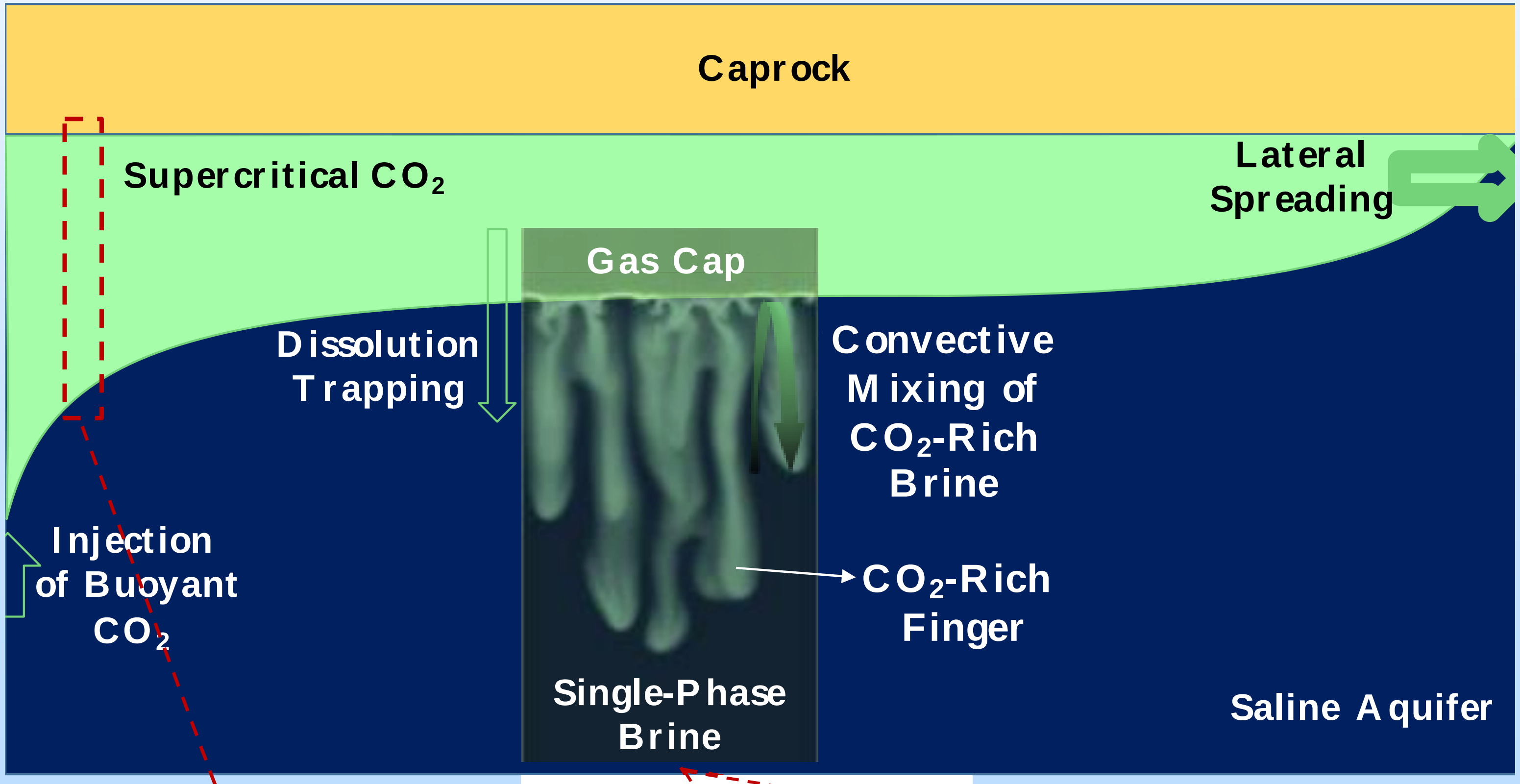
Tasks

1. Numerical modeling of reactive transport at Cranfield and Chester 16 CCS Site(s) to
   - *Better interpret field data*
   - *Predict long-term evolution of fluids & formation*
   - *Apply lessons learned to other projects*
2. Assess efficiency of PFT analysis using capillary adsorption tubes in a hydrocarbon-rich matrix

Task 1 Objective

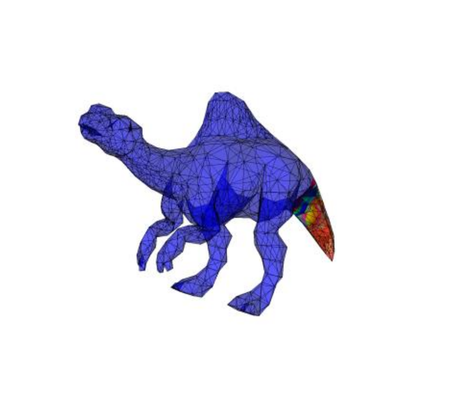
- Constrain **structural, solubility, and chemical** trapping mechanisms that guarantee storage permanence, through novel subsurface signals & modeling.
  - Non-trivial migration patterns in heterogeneous formations
  - Diffusion driven convection and cross-flow into low-perm. facies
  - Chemically driven mineralization of CO_2 and formation alterations

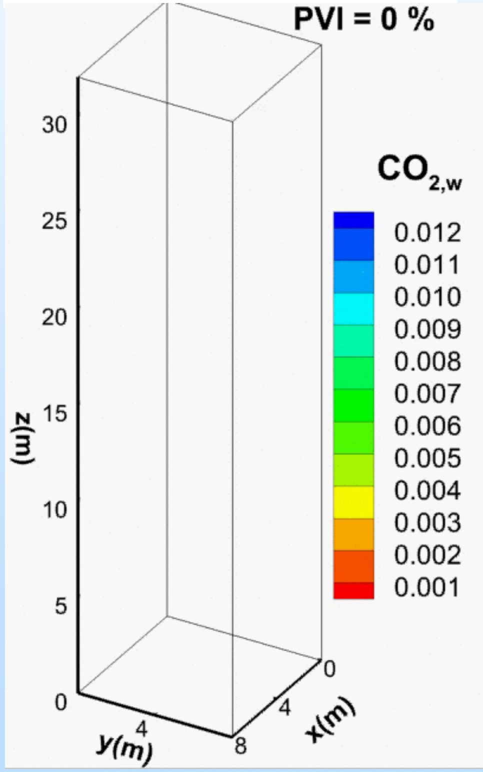
- Iteratively coupled workflow of field data and modeling



Modeling Tools

- Unique combination of capabilities in **Osures**:
  - Higher-order finite element (FE) methods for flow and transport: allow unstructured grids, tensor permeability, discrete fractures, heterogeneity
  - Low numerical dispersion (e.g., resolves small-scale onset of instabilities)
  - Cubic-plus-association (CPA) equation of state (non-ideal) phase behavior modeling of water, CO_2, hydrocarbons, tracers (capture, e.g., competitive dissolution and brine compressibility)
  - Fickian diffusion with self-consistent composition + T + p -dependent full matrix of diffusion coefficients for multicomponent multiphase fluids
  - Capillary-driven flow with composition + p -dependent surface tension
  - ***New*** Reactive transport by coupling to iPHREEQC geochemistry (2019-2020) and **PhreeqcRM** (2020-2021), which is faster / parallelizable.





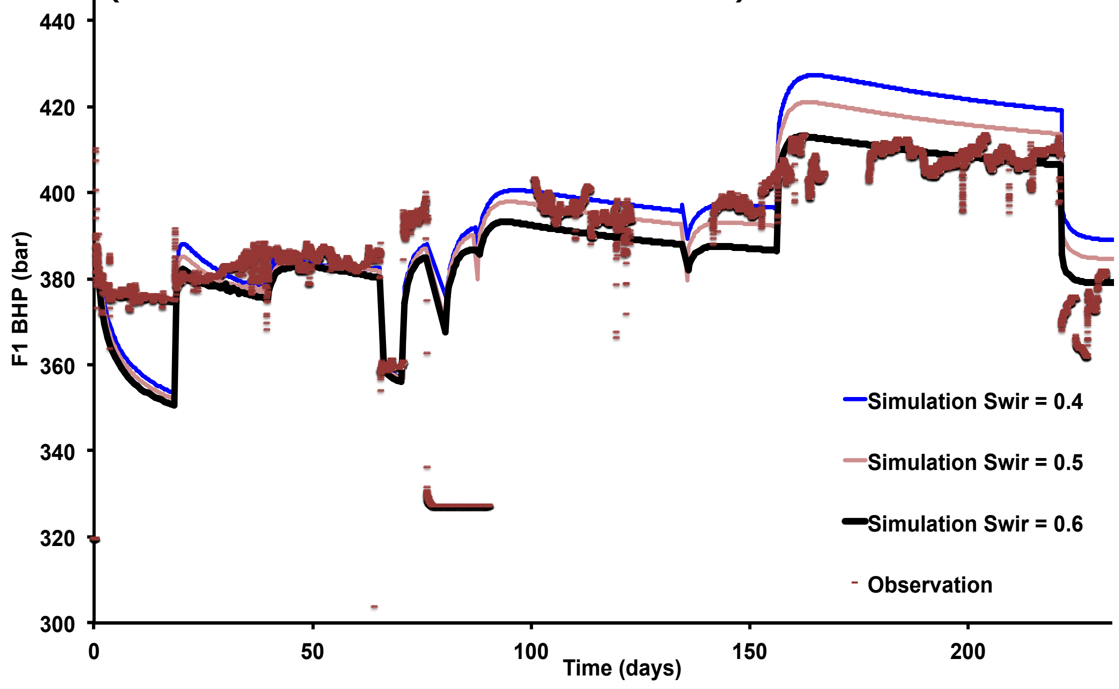
Prior Accomplishments

Modeling of pure CO_2 injection into brine at Cranfield

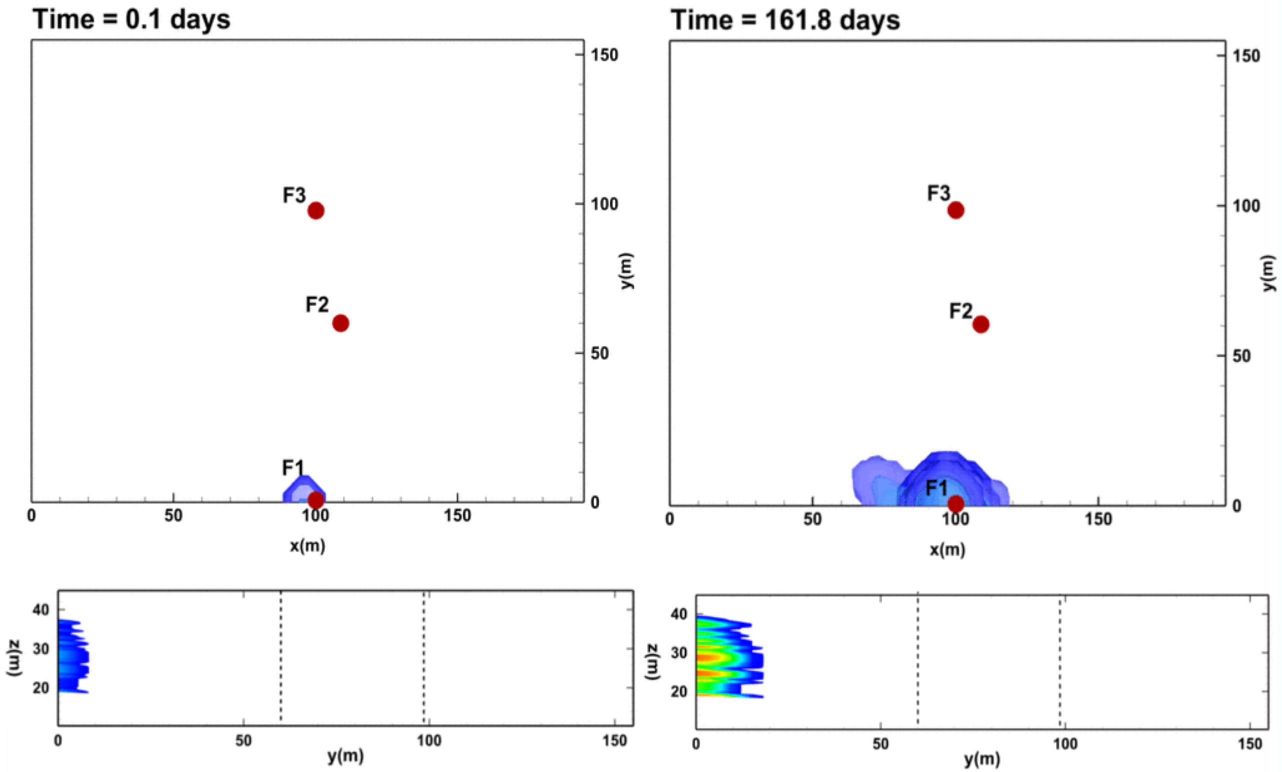
Excellent match to observed pressure response and CO_2 breakthrough times in observation wells

Pressure response in injection well

(Soltanian et al., *IJGGC* 2016)



CO_2 migration in 2009 (left) & 2010 (right)

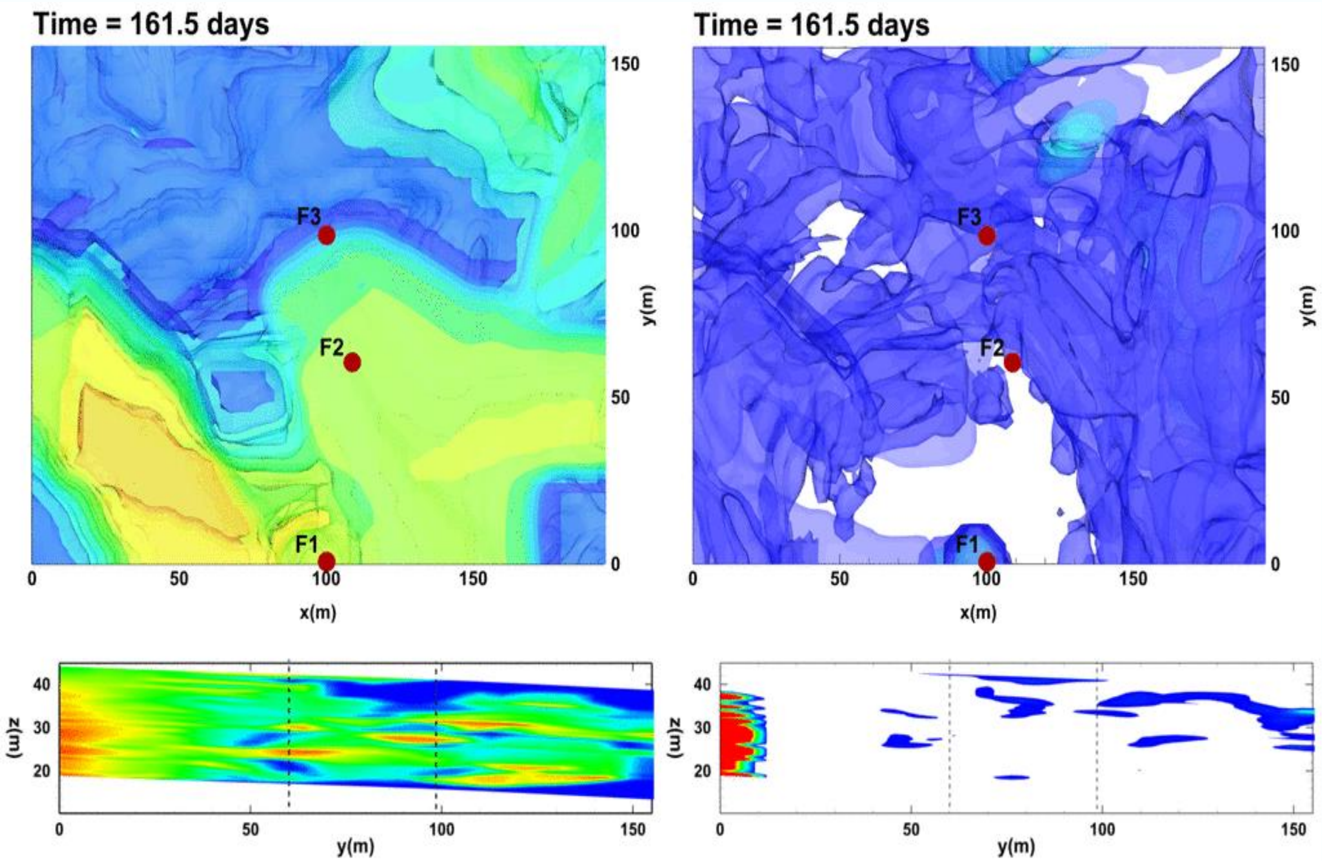


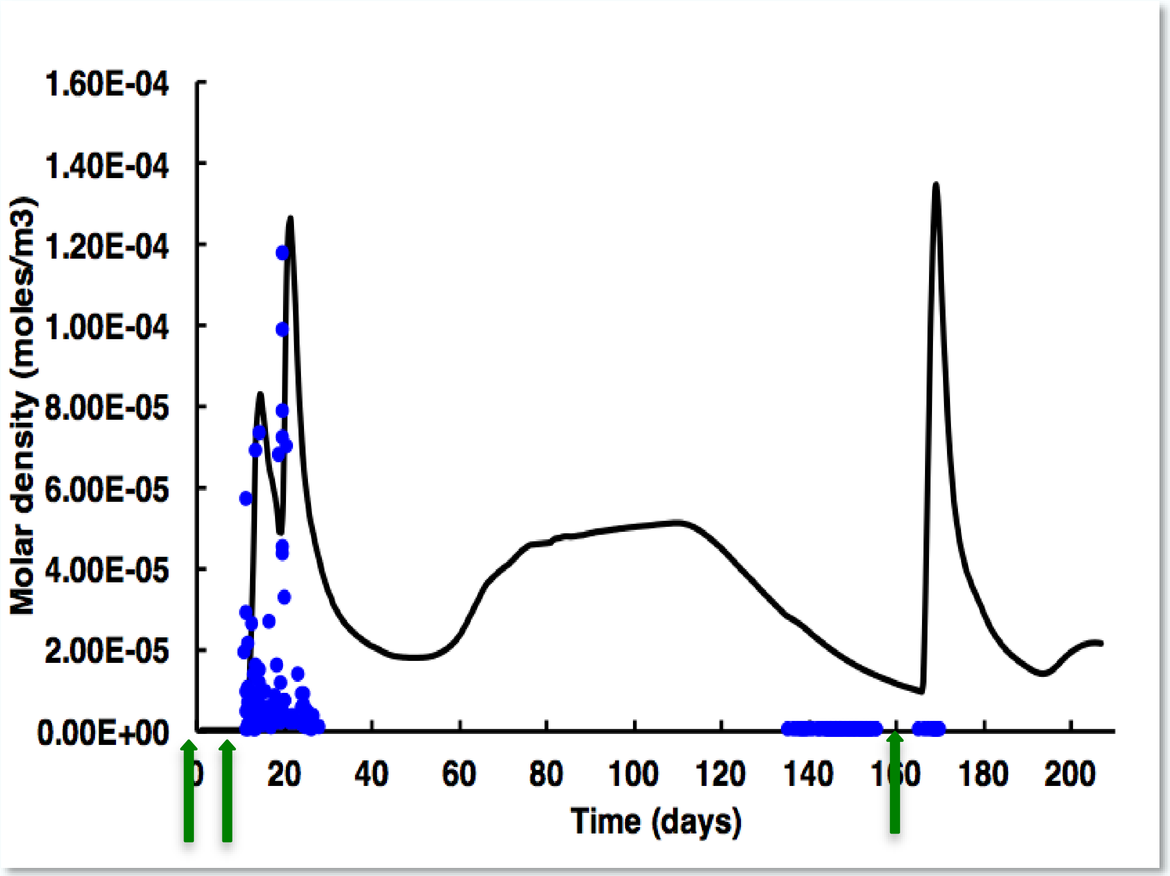
Prior Accomplishments

Modeling of perfluorocarbon tracers co-injected with CO_2

Remarkable match to breakthrough curves (at exceedingly low concentrations)

CO_2 and PFT migration (Soltanian et al., *GGST* 2018)

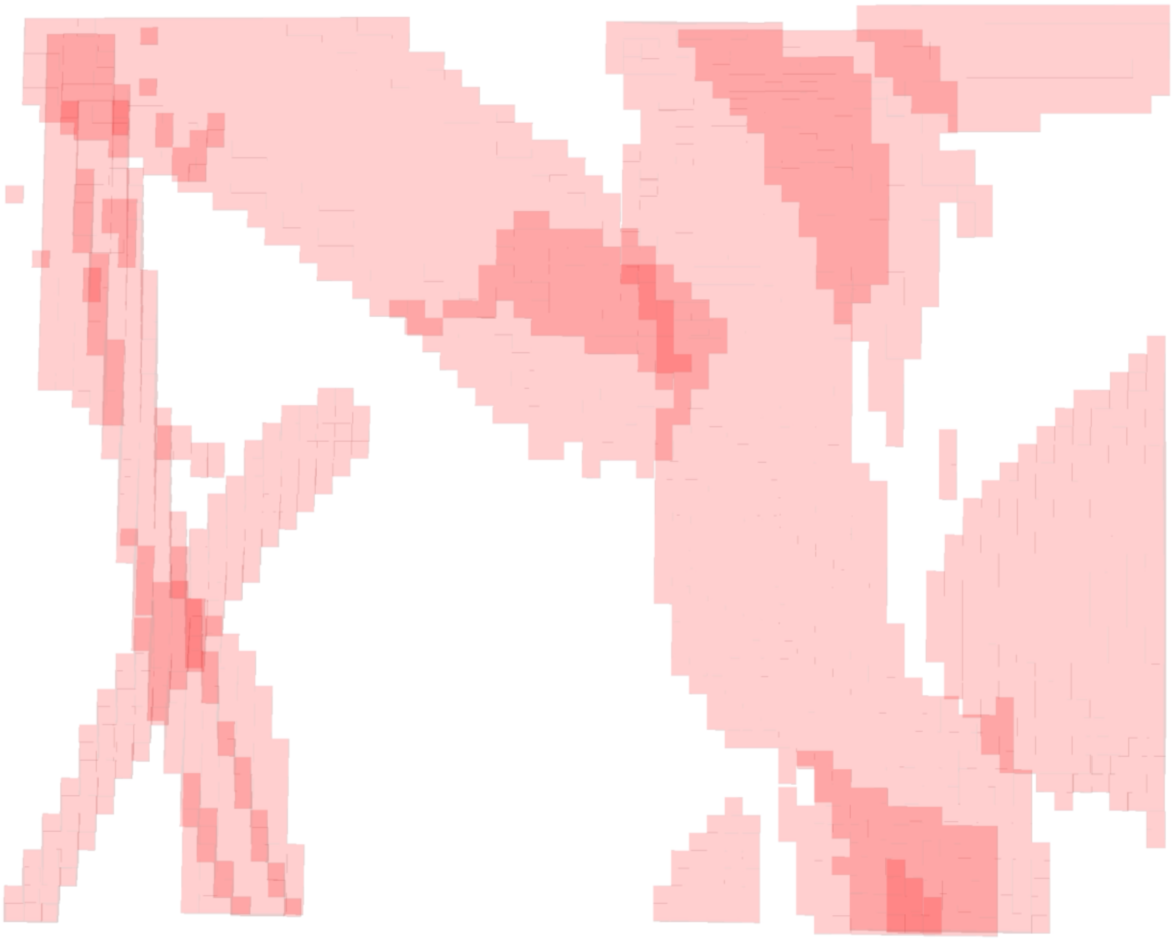


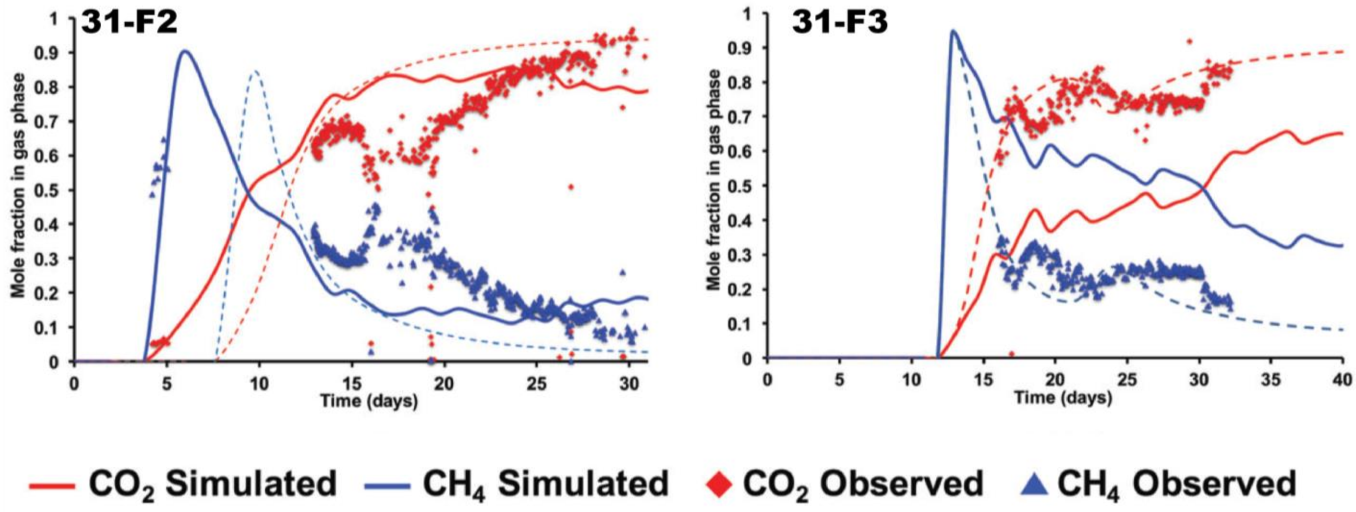


Prior Accomplishments

Modeling of the exsolution of methane dissolved in formation brine

Match to observed breakthrough curves (Soltanian et al., *Groundwater* 2018)

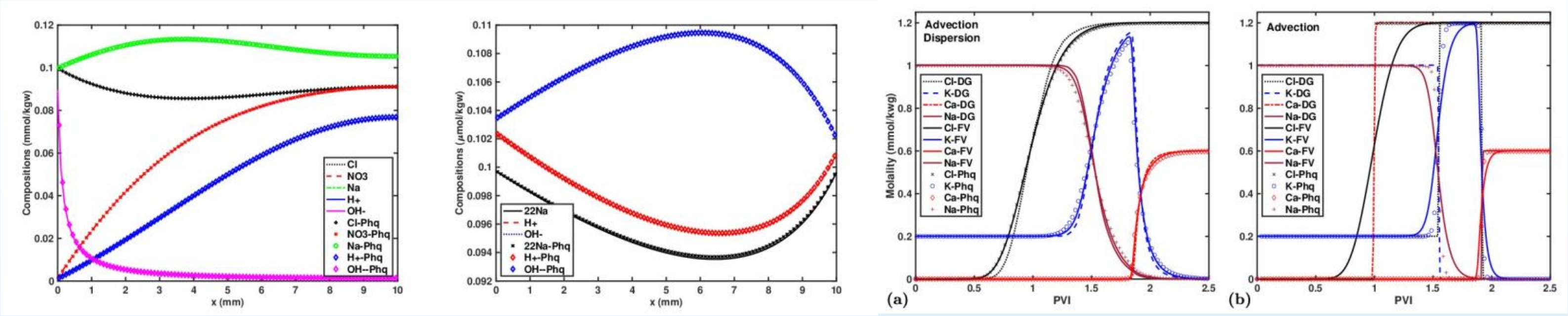




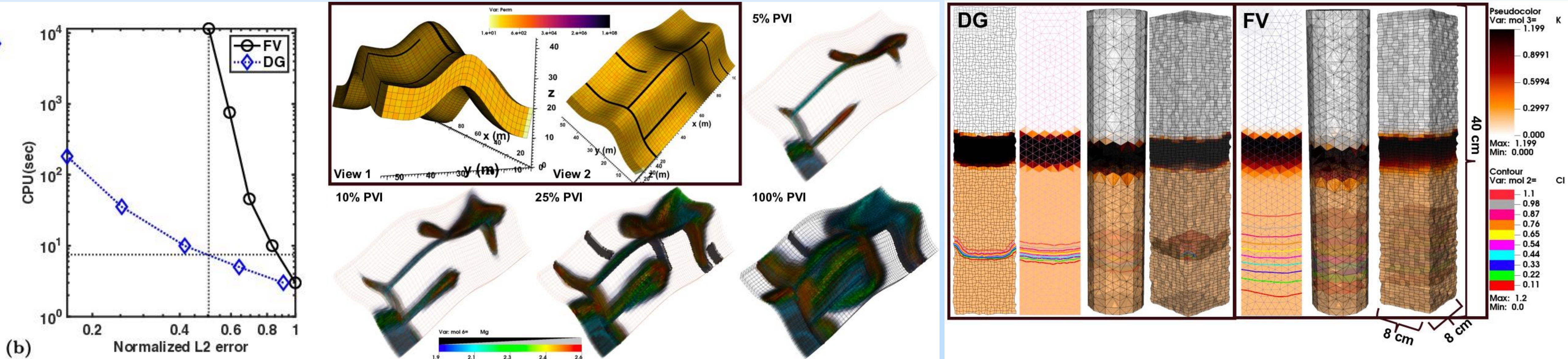
Prior Accomplishments

2020: Reactive transport by coupling to iPhreeqc and PreeqcRM interfaces, only single-phase

Excellent agreement to benchmark studies and experimental results:



but now with advanced numerical methods and more physics (Moortgat et al. *Sci Rep* 2020):



Technical Status

Two main accomplishments on Task 1 in 2021:

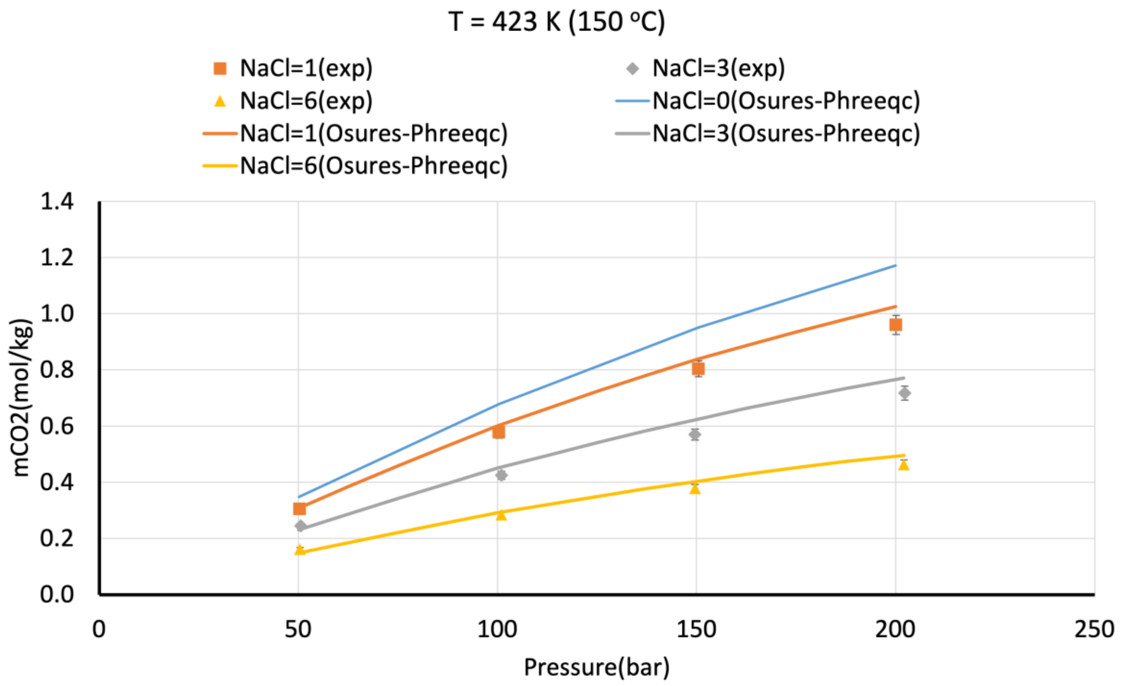
- Development of **two-phase** reactive transport with full equation-of-state based multi-component phase-split computations.

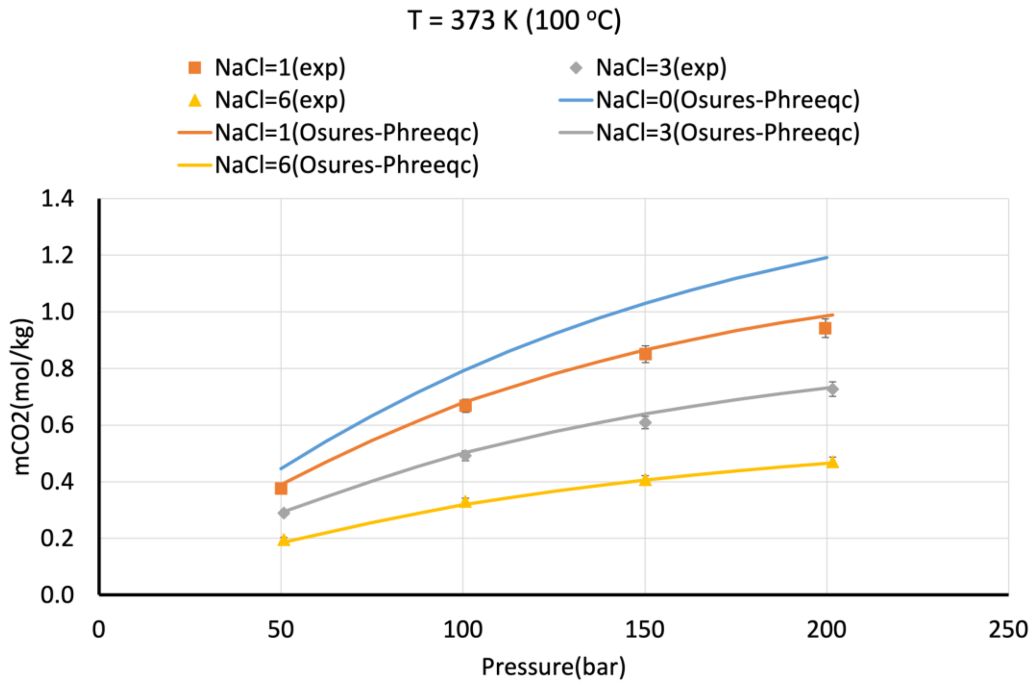
- Initial modeling of CO_2 transport in challenging **Chester 16** reef system.

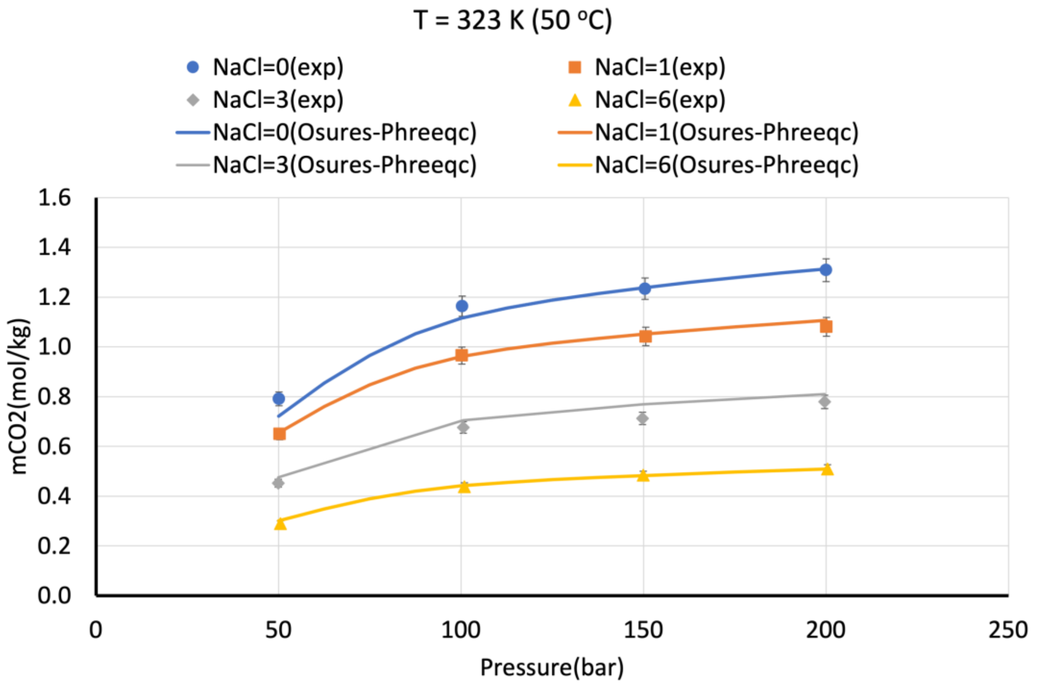
Two-Phase Geochemistry

New reactions + EOS phase-split computation formalism that strictly satisfies thermodynamic equilibrium

Effect of dissolved salts on CO_2 solubility, compared to experimental data

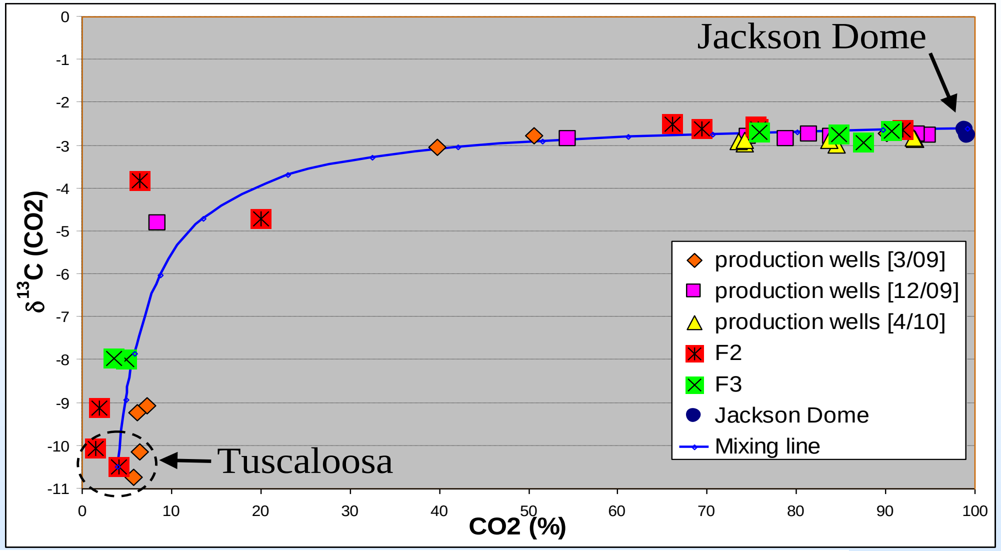




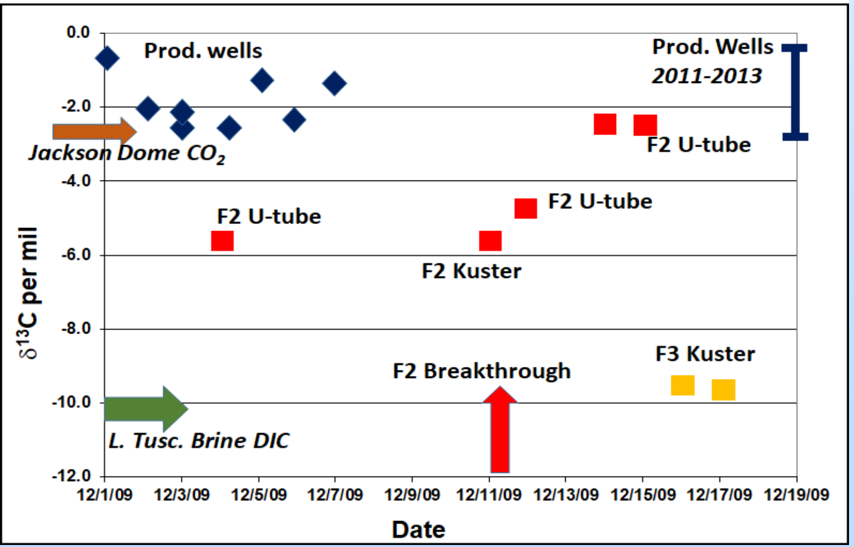


Two-Phase Geochemistry

Carbon isotope evidence for mixing of formation CO_2 with injectate

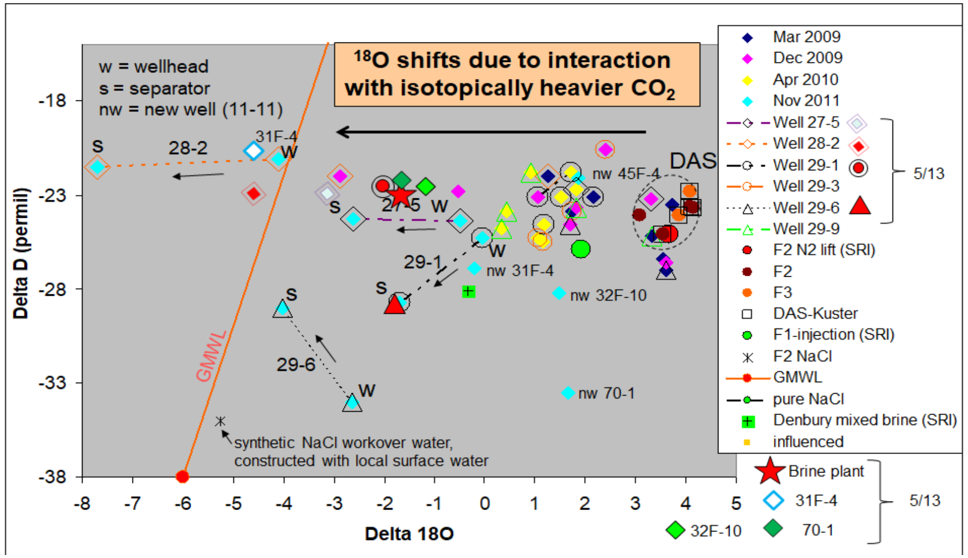


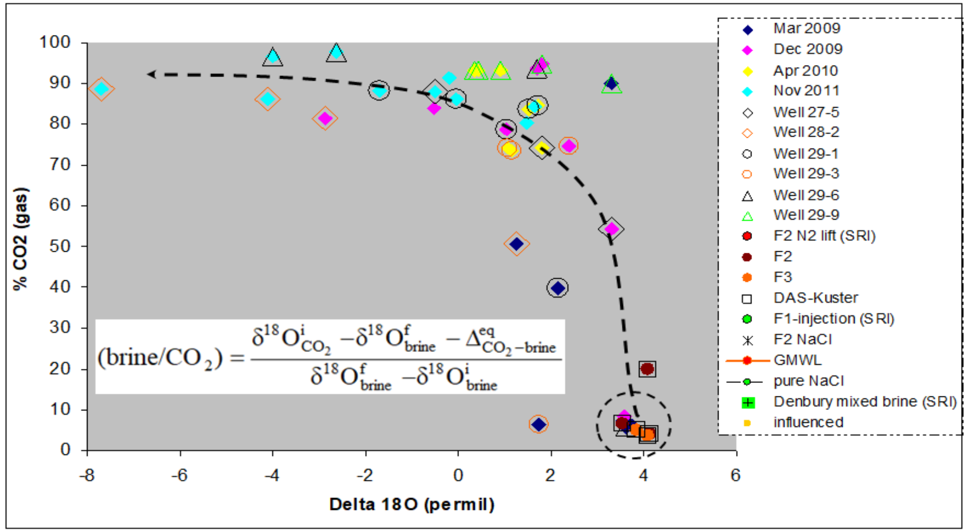
Dissolved Inorganic Carbon (DIC)



Carbon isotope evolution of DIC in DAS and production wells from pre- to post-breakthrough

Oxygen isotope shift in brines reveals the fraction of CO_2 "communicating" with fluid

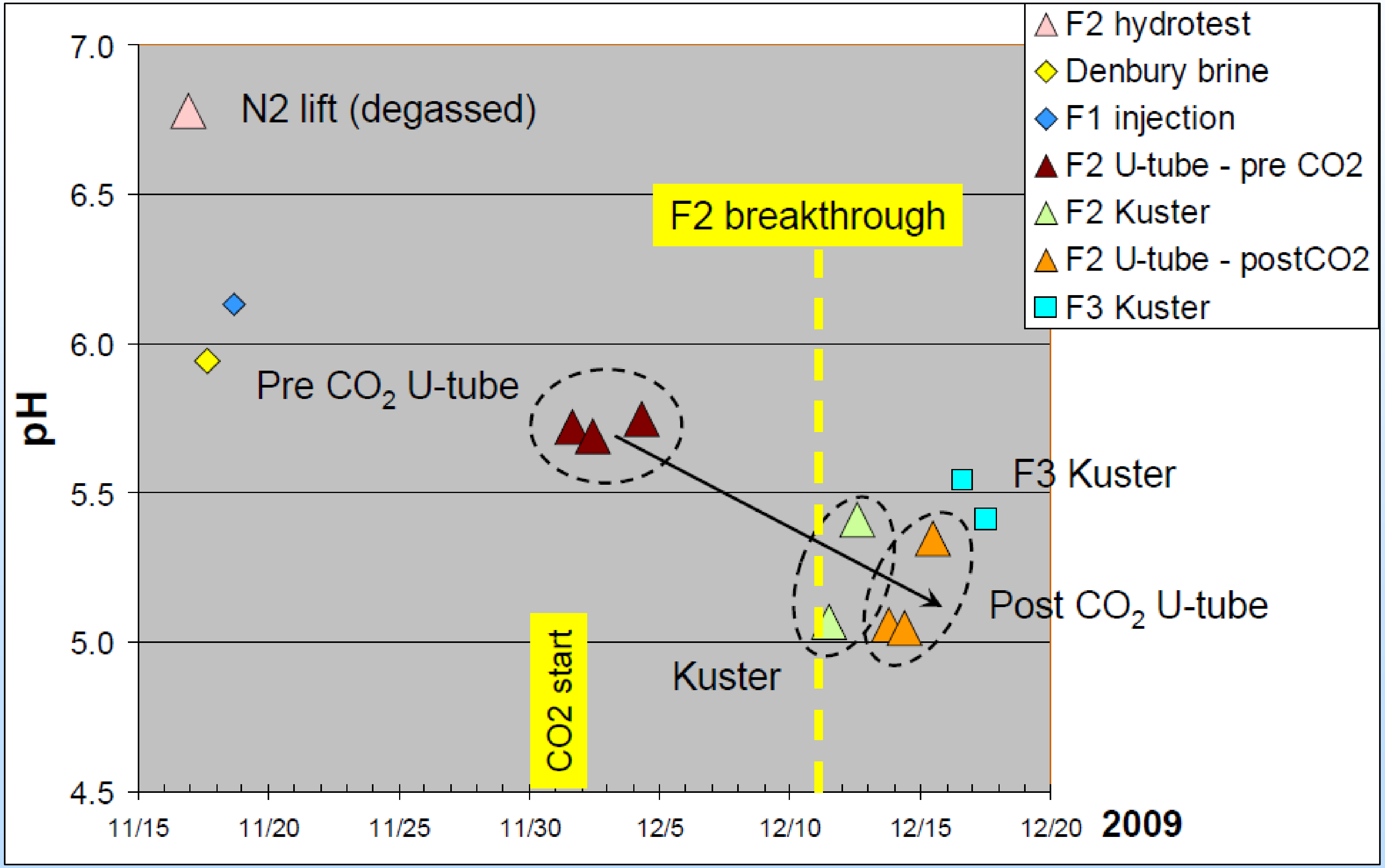




$$(\mathrm{brine}/CO_2) = \frac{\delta^{18}O^{i}_{CO_2} - \delta^{18}O^{f}_{\mathrm{brine}} - \Delta^{eq}_{CO_2-\mathrm{brine}}}{\delta^{18}O^{f}_{\mathrm{brine}} - \delta^{18}O^{i}_{\mathrm{brine}}}$$

Two-Phase Geochemistry

Measured pH change in formation brine during CO_2 injection



Two-Phase Reactive Transport

Modeling of the pH change in formation brine during CO_2 injection

pH Distribution

2.5	2.75	3	3.25	3.5

CO_2 injection Z_{CO_2}

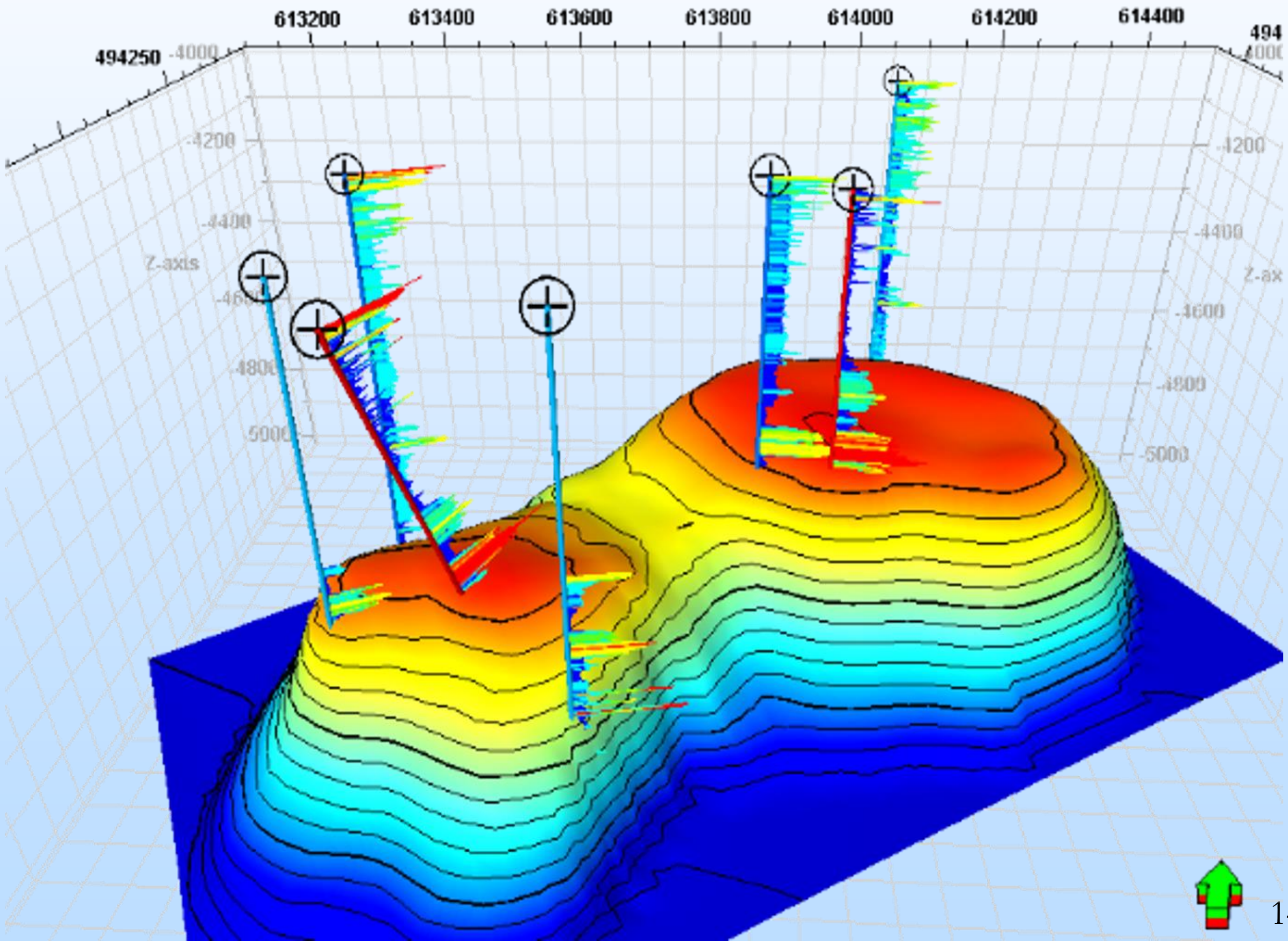
0.050	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50

Time:0

Chester 16

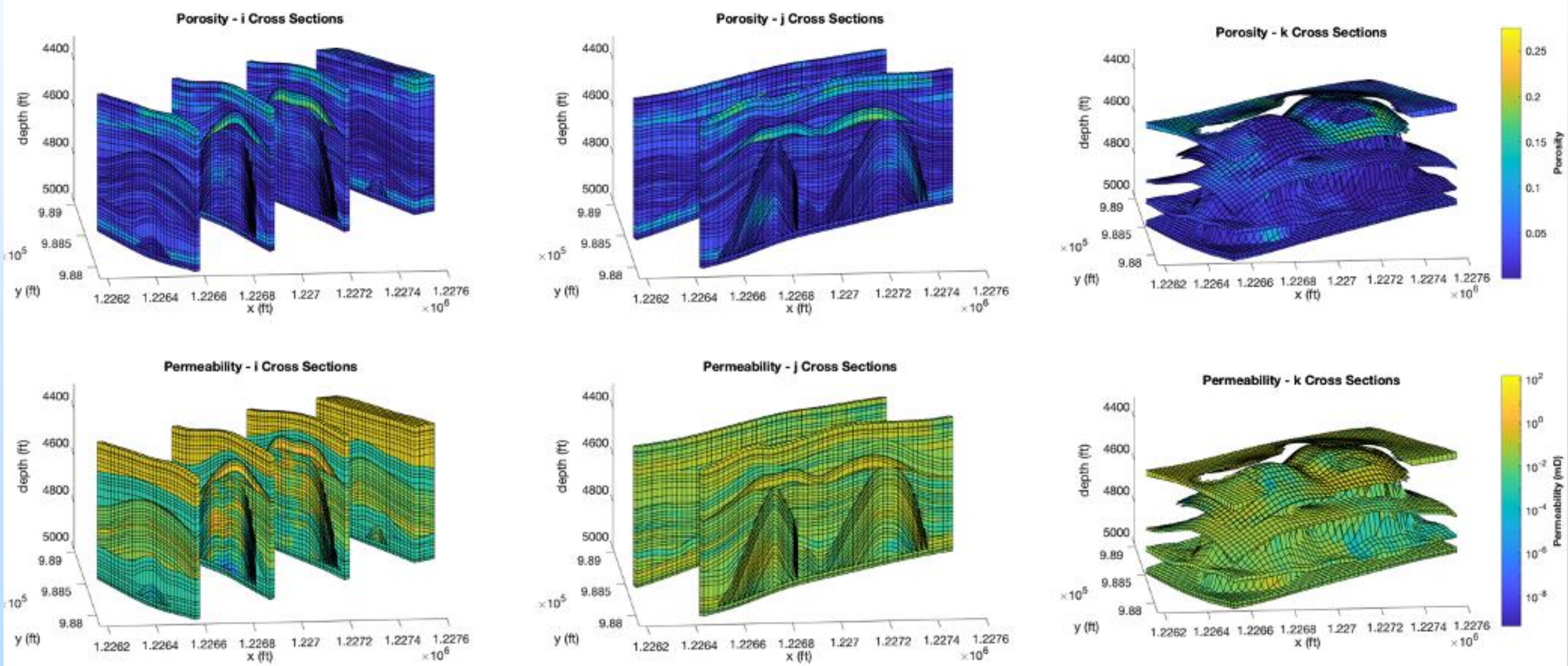
Synergistic collaboration developed with Battelle to model CO_2 transport in complex Chester 16 reef system (MRCSP)

- 2020 (and ongoing): develop alternative static models on tetrahedral grids



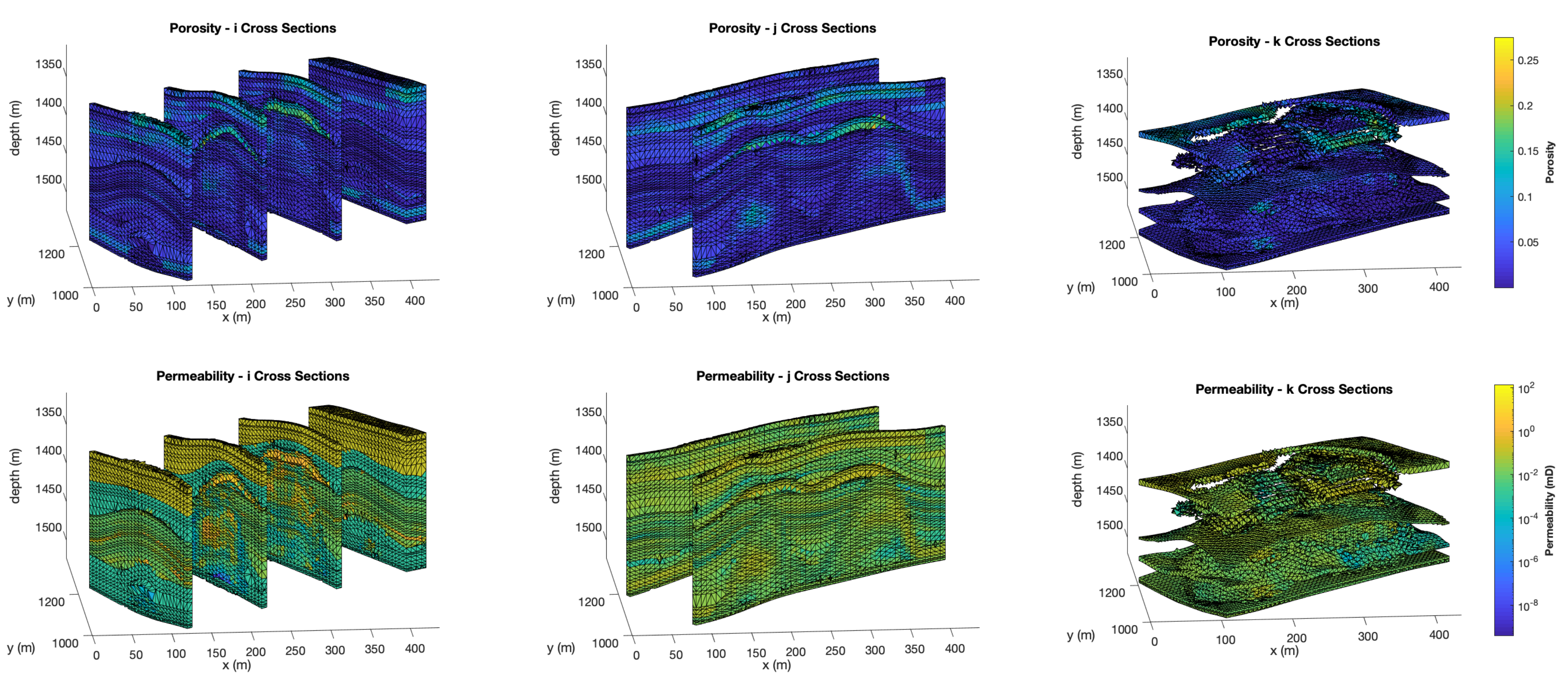
Chester 16

- Industry-standard is logically Cartesian corner-point grids
- For complex geometry, like domes, many dead and pinched cells
- Can truly unstructured, e.g., tetrahedral, grids offer advantages?



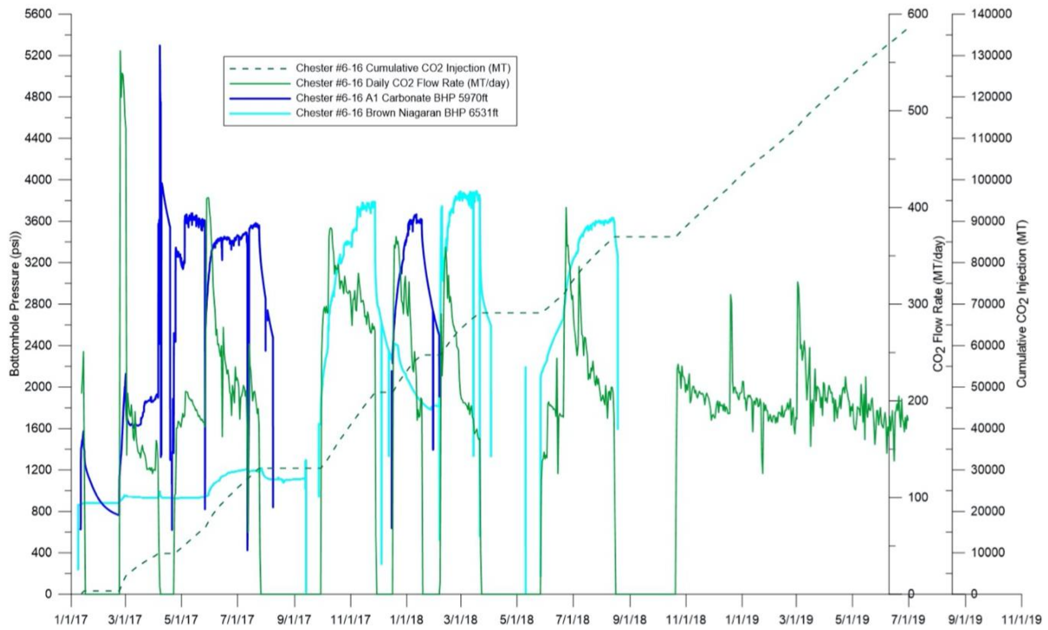
Chester 16

- Tetrahedral static model for Chester 16 reported in 2020 reports
- 361,210 tetrahedral grid elements, 1,250 m × 700 m × 215 m



Chester 16

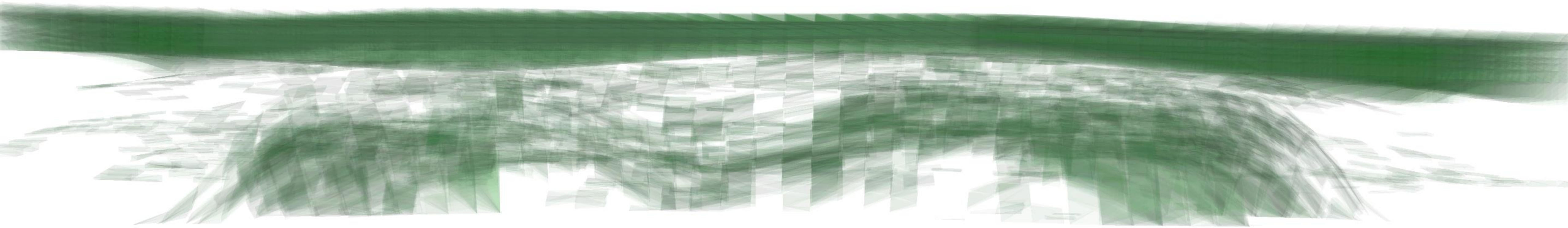
- Multiple injection and ‘soak’ periods
- Model CO_2 injection into water at BHP of 130 bar and T = 104 F where CO_2 is supercritical

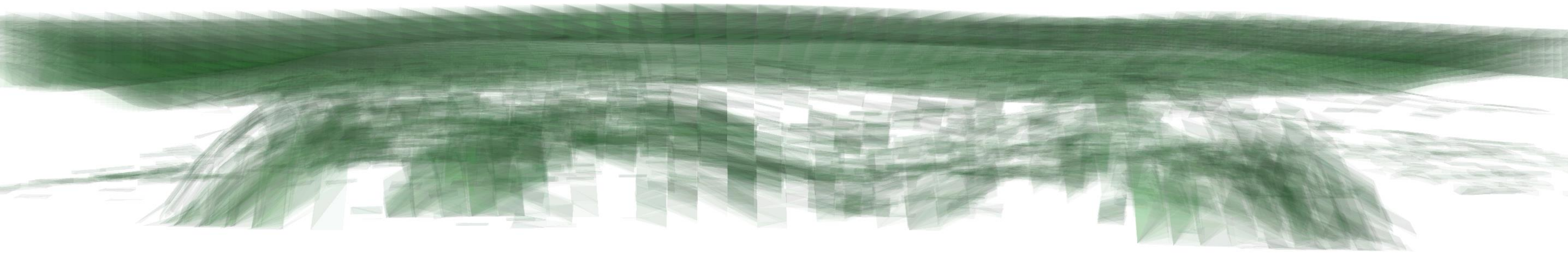


Injection Period	Date Range	Days Injected	Target Formation	CO_2 Injected (MT)
1	1/11/17 - 1/14/17	3	A1 Carbonate	804
2	2/22/2017 - 4/6/2017	43	A1 Carbonate	9,039
3	4/22/2017 - 7/24/2017	93	A1 Carbonate	20,585
4	9/29/2017 - 11/27/2017	59	Brown Niagaran	18,314
5	12/16/2017 - 1/16/2018	31	A1 Carbonate	9,010
6	2/5/2018 - 3/21/2018	44	A1 Carbonate and Brown Niagaran	10,178
7	5/26/2018 - 8/14/2018	80	A1 Carbonate and Brown Niagaran	18,320
8	10/20/2018 - 7/29/2019	Continuing	A1 Carbonate and Brown Niagaran	55,390

Chester 16

- Preliminary modeling of CO_2 injection (higher-order DG)
- Two viewing angles, 1 year of injection, 1 mol% CO_2 contours (and perm.)





Lessons Learned

- (Task 2) Perfluorocarbon and isotope tracers offer powerful tools to track migration of injected CO_2 through arrival times and breakthrough curves in observation/production wells, measure degree of mixing with brine.

- (Task 1) Numerical models have matured enough to match and interpret field data and make predictions for future CO_2 storage projects.

- (Task 1) Predictive capabilities sensitive to accuracy of static models, i.e., capturing formation heterogeneity, and relative permeability / capillarity relations, which are generally facies dependent.

Project Summary (Task 1)

- Completed:
  - Modeling of CO_2, CH_4, brine, and perfluorocarbon tracers at Cranfield
  - Fundamental analyses of solubility trapping (mixing and spreading of dissolved CO_2)
  - Initial implementation and benchmarking of coupled flow and reactive transport with Osures+iPhreeqc/PhreeqcRM

- Ongoing & Future work:
  - Investigation of *multiphase* flow and *reactive* transport at Cranfield
  - Modeling of independent Chester 16 field site
  - Technology improvements (specifically parallelization / HCP)
  - Final summary report in April 2022

Project Summary (Task 1)

- Completed:
  - PFT and isotope tracer field experiments at Cranfield
  - Lab experiments of best practices in use of PFTs, investigating effects of hydrocarbons and improved substrates in sorbent tubes (e.g., Carbonex 569)

- Future work:
  - Final synthesis of geochemical data and PFT analysis best practices reported in April 2022

Synergies

- Established collaborative simulation opportunities with MRCSP regarding complex reef systems.
- Open to other partnerships, incl. future large-scale projects.
- Addressing priority research directions:
  - PRD S-1: Advancing Multiphysics and Multiscale Fluid Flow to Achieve Gton/yr Capacity
  - PRD S-2: Understanding Dynamic Pressure Limits for Gigatonne-scale CO_2 Injection
  - PRD S-6: Improving Characterization of Fault and Fracture Systems
- Collaborative PFT sorbent testing in hydrocarbon-rich matrices. GC-MS experiments with NETL RIC.
- Sharing best practices for tracer analysis
  - Potential applications for CCUS Research Priority areas: Locating, Evaluating, and Remediating Existing and Abandoned Wells & Wellbore leakage

APPENDICES

Organization Chart

U.S. DEPARTMENT OF ENERGY | NETL

OAK RIDGE National Laboratory

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Postdocs: Soltanian, Zhu, Li

Collaborators:

NATIONAL ENERGY TECHNOLOGY LABORATORY

BUREAU OF ECONOMIC GEOLOGY JOHN A. and KATHERINE G. JACKSON SCHOOL OF GEOSCIENCES

BERKELEY LAB

USGS science for a changing world

BATTELLE

Gantt Chart

Task	Milestone Description*	Fiscal Year 2019				Fiscal Year 2020				Fiscal Year 2021				Planned Start Date	Planned End Date	Actual Start Date	Actual End Date
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4				
2.1	Survey field test opportunities for enhanced PFT sampling technology	■												9/18	12/18	9/18	12/18
2.1	Thermal desorption system installed on ORNL's gas chromatography system		■	■										2/19	3/19	2/19	3/19
2.1	Sorbent selected for PFT-hydrocarbon experiments		■	■										3/19	6/19		7/19
1.1	Initial transport modeling of aqueous equilibrium reactions with Osures+iPhreeqc	■	■	■	■									3/19	9/19	3/19	9/19
1.2	Data sharing planned with partner institution(s) for future modeling of a CCS project independent of the Cranfield DAS		■	■	■	■								3/19	12/19		12/19
2.1	Validation of PFT sorbent sampling method in hydrocarbon matrices				■	■	■							7/19	12/19		3/20
2.1	Best practices identified for PFT sampling in hydrocarbon-rich environments					■	■	■	■					9/19	12/20		
1.2	Static model developed for a modeling benchmark study of an independent CSS project				■	■	■	■						7/19	6/20		8/20
1.1	First demonstrations of reactive transport modeling of the multiphase brine-CO_2-rock system using higher-order accurate methods				■	■	■	■	■	■				7/19	12/20		
1.2	Modeling of CO_2-brine flow and transport for a field site different from Cranfield DAS						■	■	■	■	■			1/20	3/21		
1.1	Final model of geochemistry and reactive transport at Cranfield								■	■	■	■		7/20	6/21		
1.1	Complete CO_2-brine-rock geochemistry and reactive transport incorporated into CSS simulations									■	■	■	■	10/20	9/21		
3	Final report on Monitoring of Geological CO_2 Sequestration Using Isotopes and Perfluorocarbon Tracers						■	■	■	■	■	■	■	1/20	9/21		