Optimal Model Complexity in Geological Carbon Sequestration: A Design of Experiment (DoE) & Response Surface (RS) Uncertainty Analysis

Project Number: DE-FE-0009238

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U.S. Department of Energy
National Energy Technology Laboratory
Carbon Storage R&D Project Review Meeting
Developing the Technologies and
Infrastructure for CCS
August 12-14, 2014

Presentation Outline

- Project goals and benefits;
- Detailed project objectives & success criteria;
- Accomplishments to date;
- Summary of results;
- Appendix (organization chart; Gantt chart; supplemental results).

Benefit to the Program

Major goals:

Support industry's ability to predict CO_2 storage capacity in geologic formations to within ±30% accuracy;

Develop and validate technologies to ensure 99% storage permanence.

Project benefits:

Facilitate the development and implementation of efficient workflows for modeling field-scale GCS in a variety of geochemically reactive environments, where formations exhibit multiple scales of permeability (*k*) heterogeneity.

Project Overview: Goals and Objectives

- Develop, test, and verify the DoE and RS uncertainty analysis for a fully heterogeneous reference model (FHM) & increasingly lower resolution “geologic models” created from upscaling the FHM.

- Investigate the effect of increasing reservoir *k* variance and depth on the uncertainty outcomes including optimal heterogeneity resolution(s). At greater injection depths, investigate gravity-stable injection.

- Investigate the effect of mineral reactions on GCS, including mineral volume fractions, reactive rate constants, reactive surface areas, and the impact of different geochemical databases.

Project Overview:
Success Criteria

- At increasing depth, for both weakly and strongly heterogeneous systems, the geologic models can capture the FHM CO_2 behaviors within the full parameter space; → Reduced characterization cost;

- RS analytical models are successfully verified against full-physics reservoir simulations via HPC, thus prediction uncertainty of any outcome at any time can be assessed using the low-resolution model(s) running the efficient RS models. → Enhanced computation efficiency;

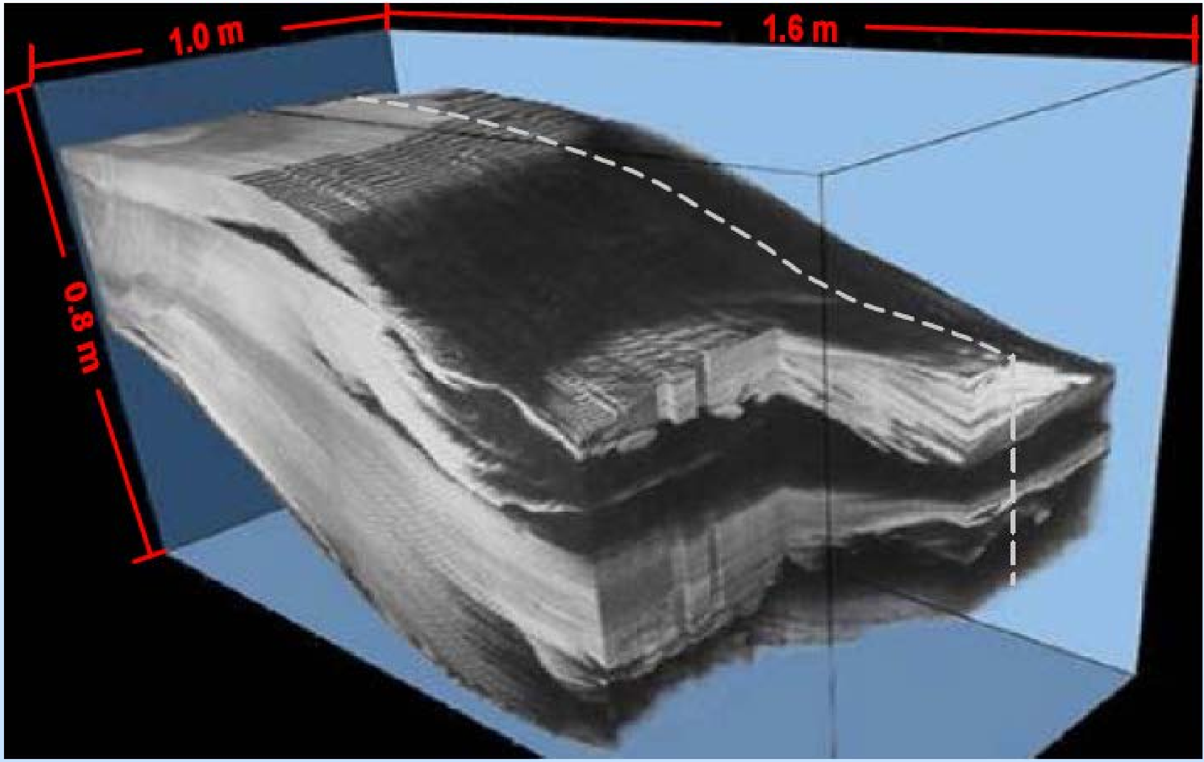
- Mineral storage analysis: seeking the most efficient composition for reactive storage → Enhanced storage;

- Greater injection depth: within the uncertainty analysis framework, identify the combination(s) of favorable parameters & reservoir condition that give rise to gravity-stable flow. → Enhanced storage security.

Accomplishments to Date

- High-resolution reservoir *k* heterogeneity (3.2 M grid cells) & geologic models of decreasing *k* resolutions;
- Permeability upscaling & single-phase flow verification;
- CO_2 modeling with PFLOTRAN & performance scaling on the petascale Yellowstone supercomputer at NWSC;
- Model comparison & DoE/RS analysis;
- CO_2 modeling considering mineral reactions.

Sediment Experiment at SAFL

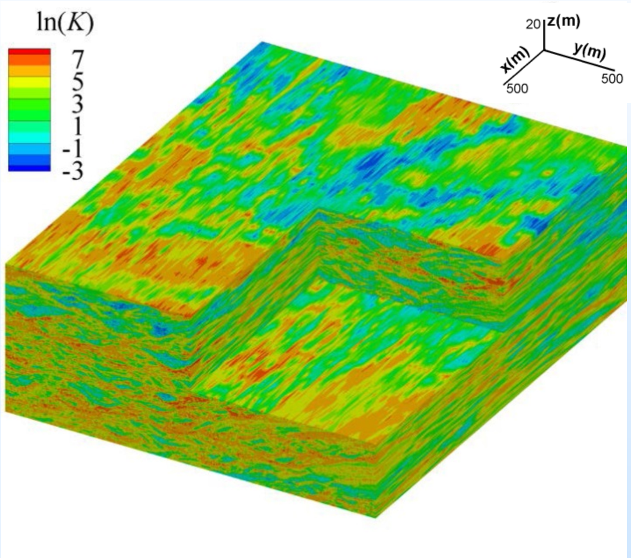


http://www.safl.umn.edu/

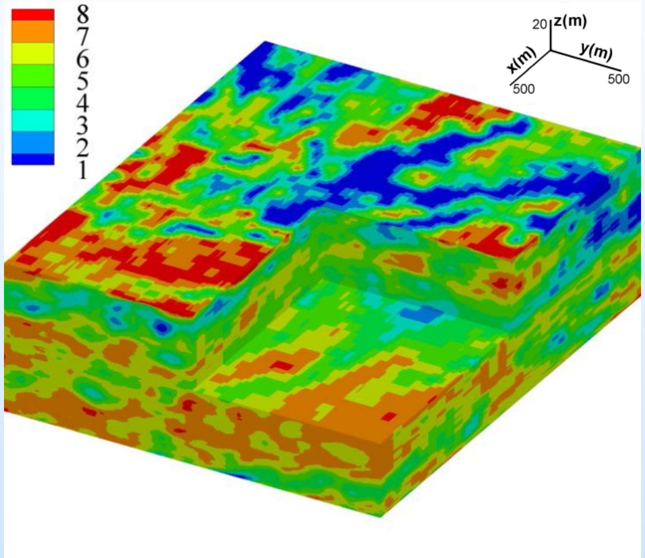
Project Leader: Prof. Chris Paola

Founding: NSF & oil industry consortium

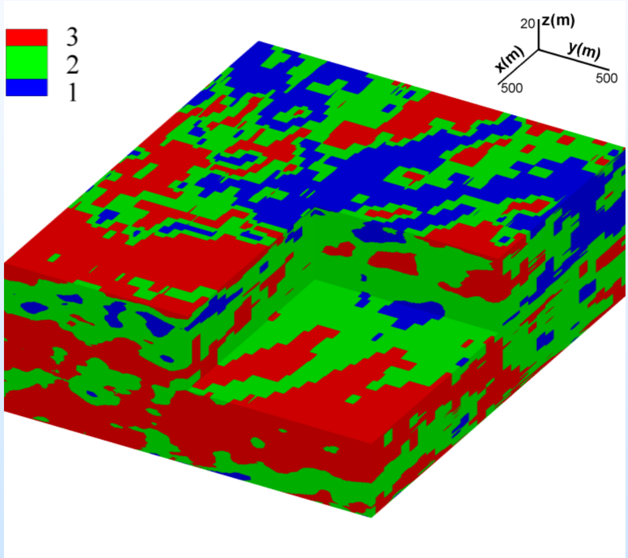
Reservoir Heterogeneity Vs Geologic Models



FHM



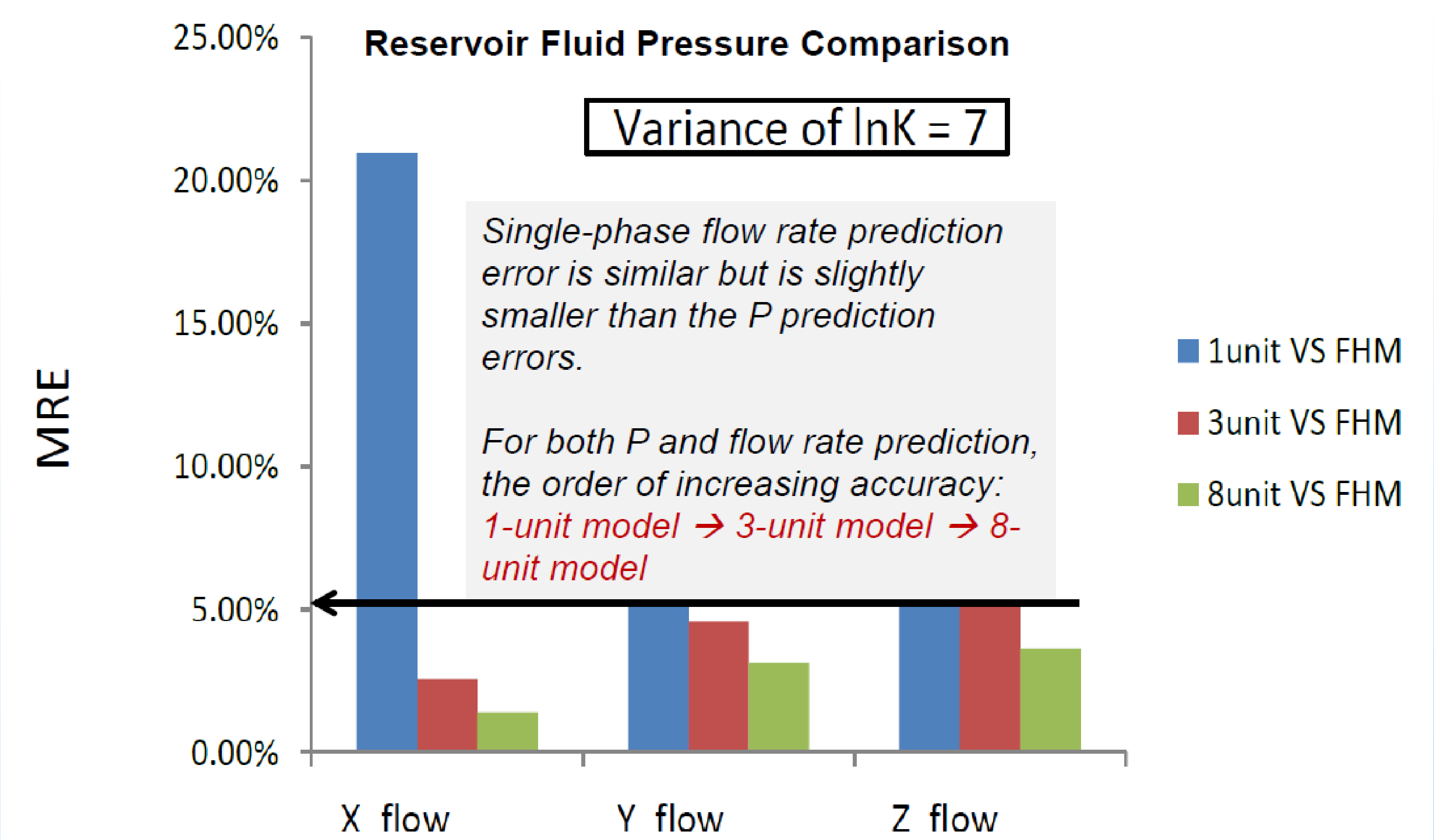
8-unit facies model



3-unit facies model

A 1-unit homogeneous “formation” model is also created (not shown);

Upscaling Verification



Single-phase flow rate prediction error is similar but is slightly smaller than the P prediction errors.

For both P and flow rate prediction, the order of increasing accuracy: 1-unit model → 3-unit model → 8-unit model

Carbon Sequestration Modeling with Reactions

- Multicomponent-multiphase non-isothermal reactive flow and transport model;
- Massively parallel---based on the PETSc parallel framework;
  - Peta-scale performance
  - Highly scalable (run on over 265k cores)
- Supercritical CO_2-H_2O;
  - Span-Wagner EOS for CO_2 density & fugacity coefficient
  - Mixture density for dissolved CO_2 in brine (Duan et al., 2008)
  - Viscosity of CO_2 (Fenghour et al., 1998)
- Finite Volume Discretization;
  - Variable switching for changes in fluid phase
  - Structured/Unstructured grids
- Reactive transport modeling, including CO_2-mineral reactions with many degrees of freedom

PFLOTRAN Scaling on Yellowstone

Yellowstone is a 1.5-petaflops supercomputer with 72,288 processor cores & 144.6 TB of memory.

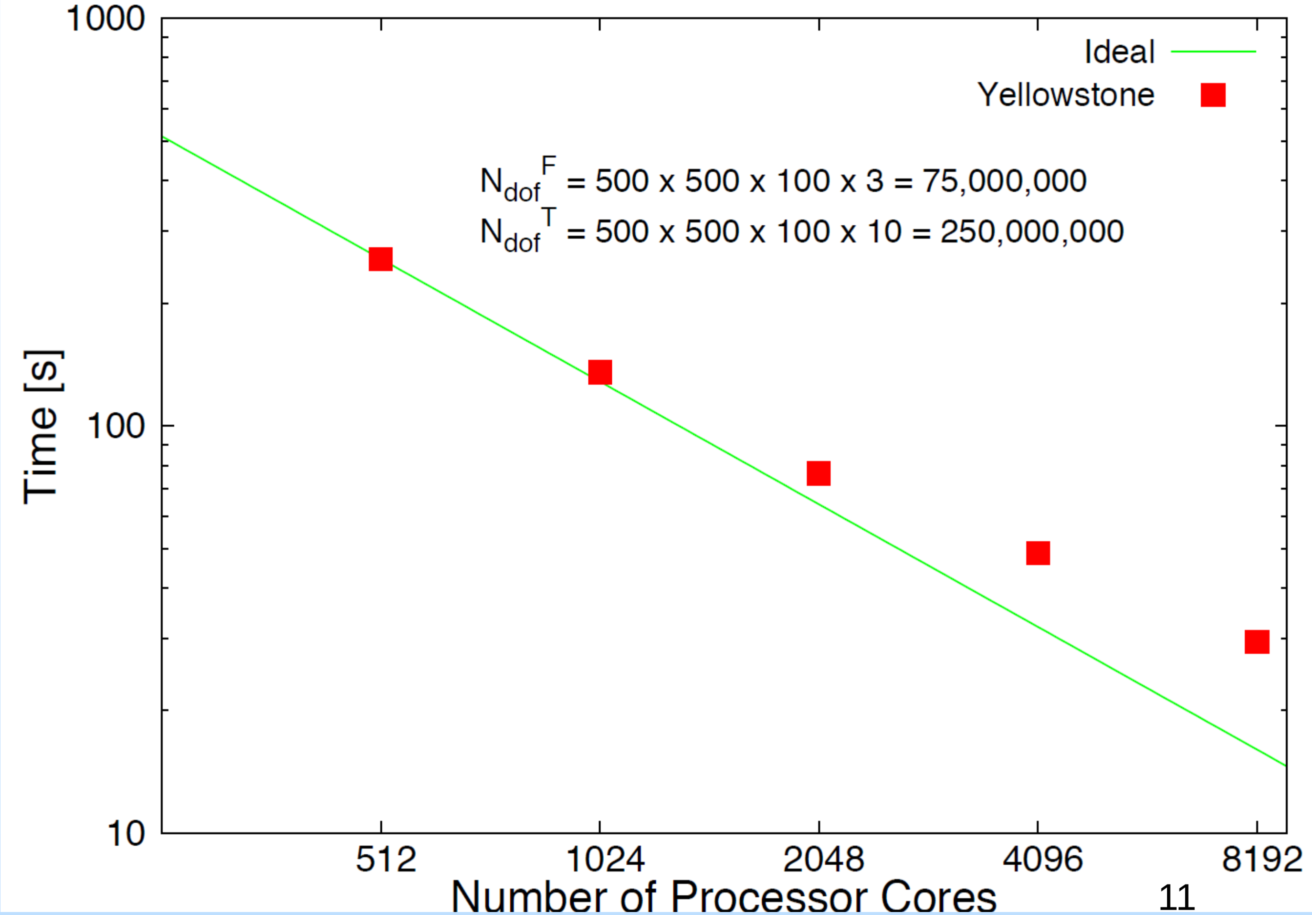
http://www2.cisl.ucar.edu/resources/yellowstone

1-unit model (3.2M):

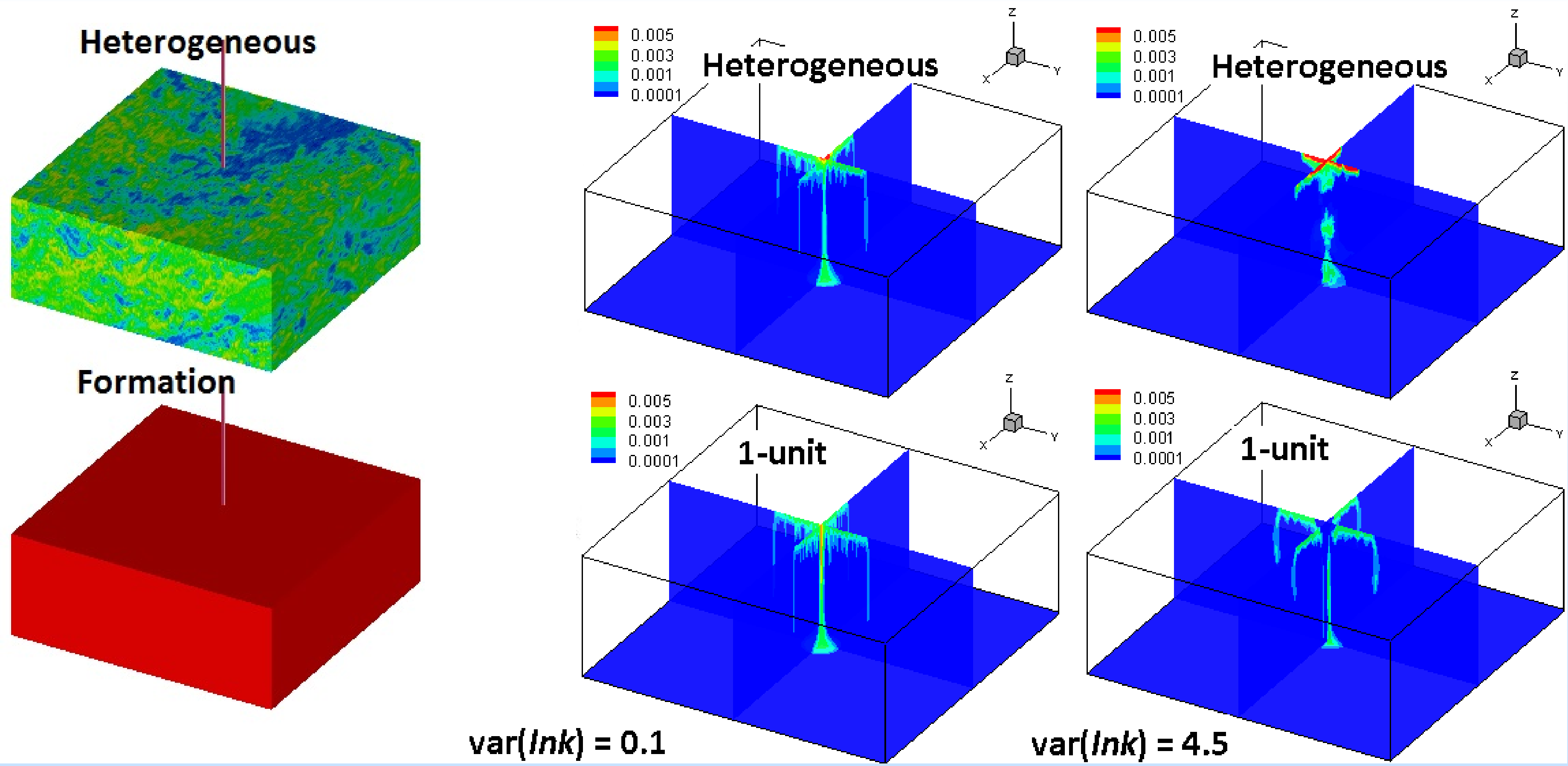
** 20 yr CO_2 injection + 2000 yr monitoring*

** 2048 cores*: 9 hours

1-unit model (25 M): CO_2 injection w/ reactive chemistry



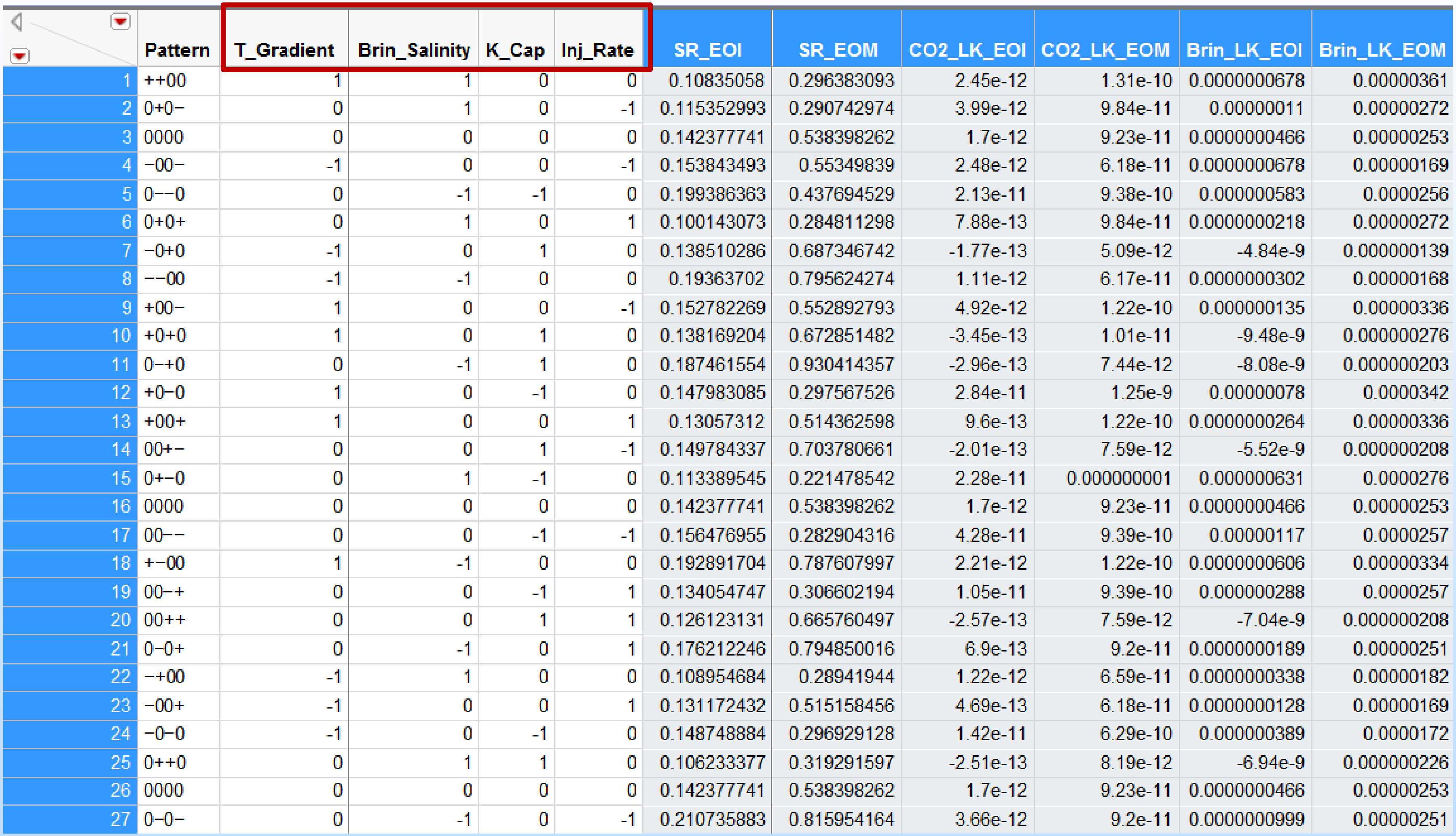
Dissolved CO_2



- Under both low and high variance conditions, the 1-unit model can reasonably capture the plume footprint of the FHM.

- Base on results of the upscaling study, the 8-unit and 3-unit models (simulations are ongoing) should yield more accurate dissolved CO_2 predictions than the 1-unit model.

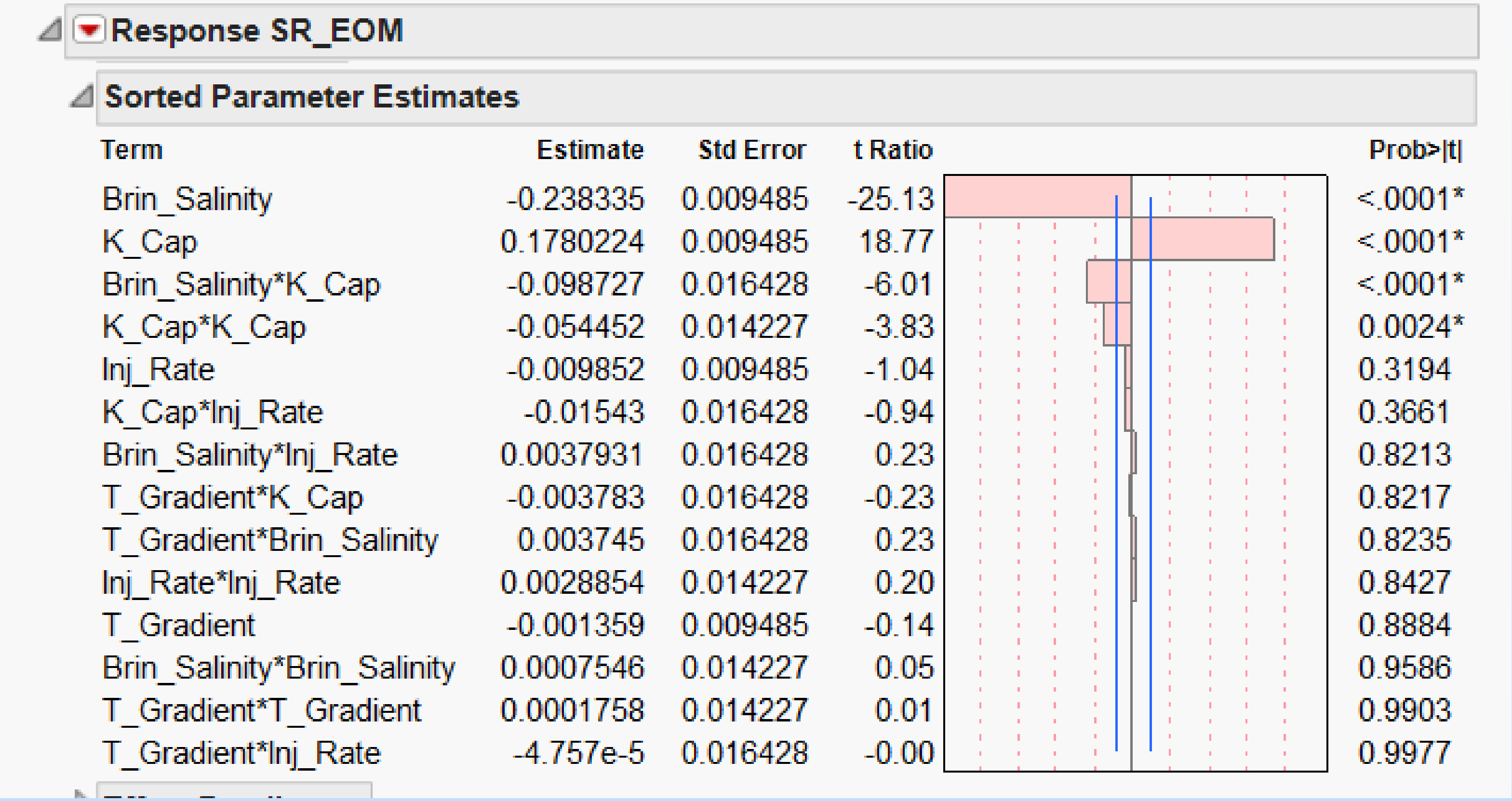
Design of Experiment (1-unit)



	Pattern	T_Gradient	Brin_Salinity	K_Cap	Inj_Rate	SR_EOI	SR_EOM	CO2_LK_EOI	CO2_LK_EOM	Brin_LK_EOI	Brin_LK_EOM
1	++00	1	1	0	0	0.10835058	0.296383093	2.45e-12	1.31e-10	0.0000000678	0.00000361
2	0+0−	0	1	0	-1	0.115352993	0.290742974	3.99e-12	9.84e-11	0.00000011	0.00000272
3	0000	0	0	0	0	0.142377741	0.538398262	1.7e-12	9.23e-11	0.0000000466	0.00000253
4	−00−	-1	0	0	-1	0.153843493	0.55349839	2.48e-12	6.18e-11	0.0000000678	0.00000169
5	0−−0	0	-1	-1	0	0.199386363	0.437694529	2.13e-11	9.38e-10	0.000000583	0.0000256
6	0+0+	0	1	0	1	0.100143073	0.284811298	7.88e-13	9.84e-11	0.0000000218	0.00000272
7	−0+0	-1	0	1	0	0.138510286	0.687346742	-1.77e-13	5.09e-12	-4.84e-9	0.000000139
8	−−00	-1	-1	0	0	0.19363702	0.795624274	1.11e-12	6.17e-11	0.0000000302	0.00000168
9	+00−	1	0	0	-1	0.152782269	0.552892793	4.92e-12	1.22e-10	0.000000135	0.00000336
10	+0+0	1	0	1	0	0.138169204	0.672851482	-3.45e-13	1.01e-11	-9.48e-9	0.000000276
11	0−+0	0	-1	1	0	0.187461554	0.930414357	-2.96e-13	7.44e-12	-8.08e-9	0.000000203
12	+0−0	1	0	-1	0	0.147983085	0.297567526	2.84e-11	1.25e-9	0.00000078	0.0000342
13	+00+	1	0	0	1	0.13057312	0.514362598	9.6e-13	1.22e-10	0.0000000264	0.00000336
14	00+−	0	0	1	-1	0.149784337	0.703780661	-2.01e-13	7.59e-12	-5.52e-9	0.000000208
15	0+−0	0	1	-1	0	0.113389545	0.221478542	2.28e-11	0.000000001	0.000000631	0.0000276
16	0000	0	0	0	0	0.142377741	0.538398262	1.7e-12	9.23e-11	0.0000000466	0.00000253
17	00−−	0	0	-1	-1	0.156476955	0.282904316	4.28e-11	9.39e-10	0.00000117	0.0000257
18	+−00	1	-1	0	0	0.192891704	0.787607997	2.21e-12	1.22e-10	0.0000000606	0.00000334
19	00−+	0	0	-1	1	0.134054747	0.306602194	1.05e-11	9.39e-10	0.000000288	0.0000257
20	00++	0	0	1	1	0.126123131	0.665760497	-2.57e-13	7.59e-12	-7.04e-9	0.000000208
21	0−0+	0	-1	0	1	0.176212246	0.794850016	6.9e-13	9.2e-11	0.0000000189	0.00000251
22	−+00	-1	1	0	0	0.108954684	0.28941944	1.22e-12	6.59e-11	0.0000000338	0.00000182
23	−00+	-1	0	0	1	0.131172432	0.515158456	4.69e-13	6.18e-11	0.0000000128	0.00000169
24	−0−0	-1	0	-1	0	0.148748884	0.296929128	1.42e-11	6.29e-10	0.000000389	0.0000172
25	0++0	0	1	1	0	0.106233377	0.319291597	-2.51e-13	8.19e-12	-6.94e-9	0.000000226
26	0000	0	0	0	0	0.142377741	0.538398262	1.7e-12	9.23e-11	0.0000000466	0.00000253
27	0−0−	0	-1	0	-1	0.210735883	0.815954164	3.66e-12	9.2e-11	0.0000000999	0.00000251

Parameter Ranking (1-unit)

Outcome: dissolved CO_2 at End of Monitoring



Response SR_EOM

Sorted Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Brin_Salinity	-0.238335	0.009485	-25.13	<.0001*
K_Cap	0.1780224	0.009485	18.77	<.0001*
Brin_Salinity*K_Cap	-0.098727	0.016428	-6.01	<.0001*
K_Cap*K_Cap	-0.054452	0.014227	-3.83	0.0024*
Inj_Rate	-0.009852	0.009485	-1.04	0.3194
K_Cap*Inj_Rate	-0.01543	0.016428	-0.94	0.3661
Brin_Salinity*Inj_Rate	0.0037931	0.016428	0.23	0.8213
T_Gradient*K_Cap	-0.003783	0.016428	-0.23	0.8217
T_Gradient*Brin_Salinity	0.003745	0.016428	0.23	0.8235
Inj_Rate*Inj_Rate	0.0028854	0.014227	0.20	0.8427
T_Gradient	-0.001359	0.009485	-0.14	0.8884
Brin_Salinity*Brin_Salinity	0.0007546	0.014227	0.05	0.9586
T_Gradient*T_Gradient	0.0001758	0.014227	0.01	0.9903
T_Gradient*Inj_Rate	-4.757e-5	0.016428	-0.00	0.9977

Mineral List

Mineral	Formula	Init VF (%)
Quartz	SiO_2	43.04213
Calcite	$CaCO_3$	4.21872
K-Feldspar	$KAlSi_3O_8$	15.77216
Kaolinite	$Al_2Si_2O_5(OH)_4$	0
Albite	$NaAlSi_3O_8$	0
Plagioclase	$(Na_{0.75},Ca_{0.25})(Al_{1.25},Si_{2.75})O_8$	4.06691
Illite	$K_{0.6}(Mg_{0.25}, Al_{1.8})(Al_{0.5}, Si_{3.5})O_{10}(OH)_2$	4.01098
Hematite	Fe_2O_3	1.598
Dawsonite	$NaAlCO_3(OH)_2$	0
Chlorite	$(Mg_{2.5}, Fe_{2.5}, Al)(Al, Si_3)O_{10}(OH)_8$	7.191
Siderite	$FeCO_3$	0
Ankerite	$Ca(Mg_{1.3}, Fe_{0.7})(CO_3)_2$	0
Magnesite	$MgCO_3$	0
Na-Smectite	$Na_{0.290}(Mg_{0.26}, Al_{1.74})(Al_{0.03}, Si_{3.97})O_{10}(OH)_2$	0
Ca-Smectite	$Ca_{0.145}(Mg_{0.26}, Al_{1.74})(Al_{0.03}, Si_{3.97})O_{10}(OH)_2$	0
Dolomite	$(CaMg)(CO_3)_2$	0

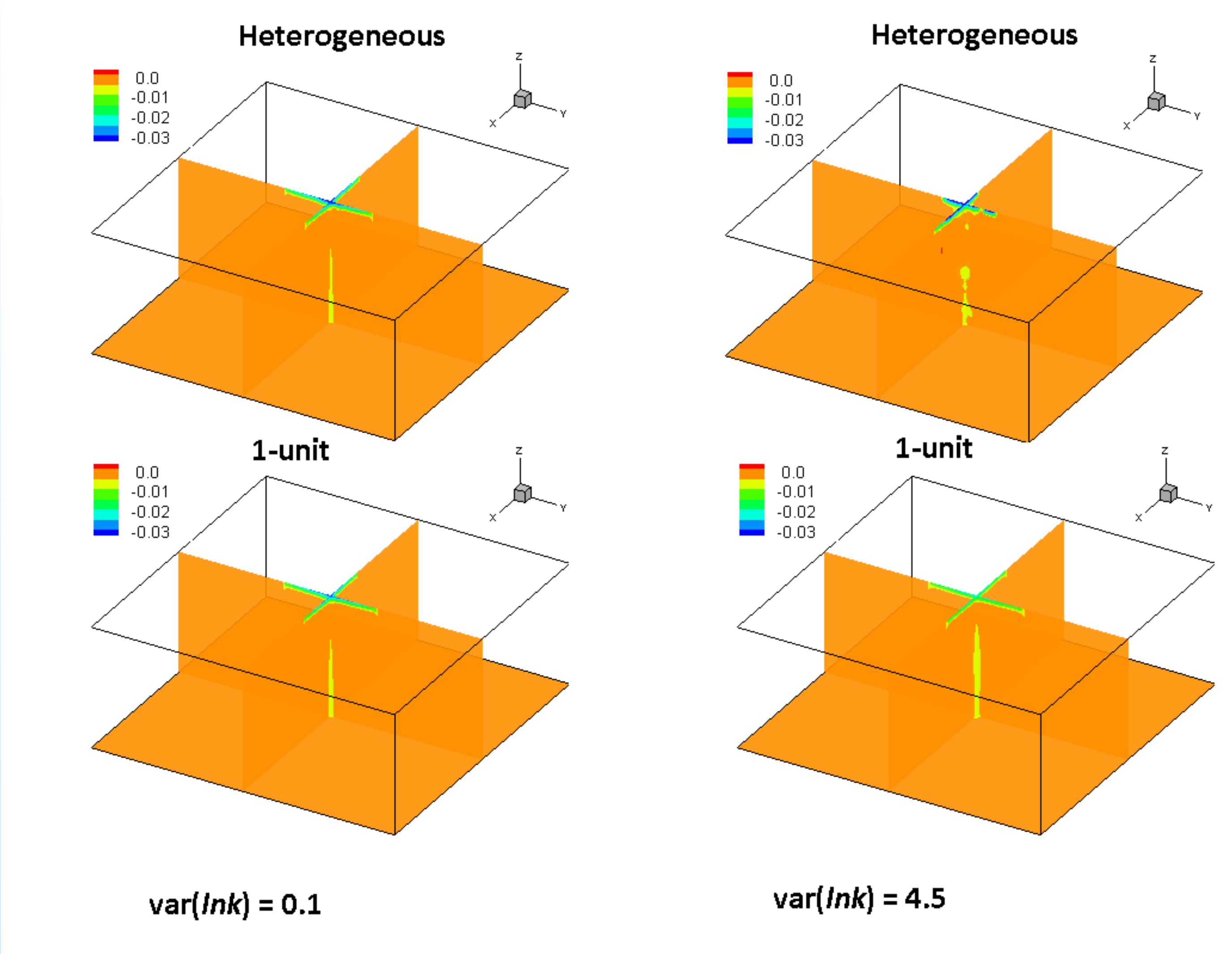
CO_2 Simulation: Mineral Trapping

- Chlorite can provide cations such as Mg^{2+} and Fe^{2+}, which are essential chemical components for forming carbonate precipitates.

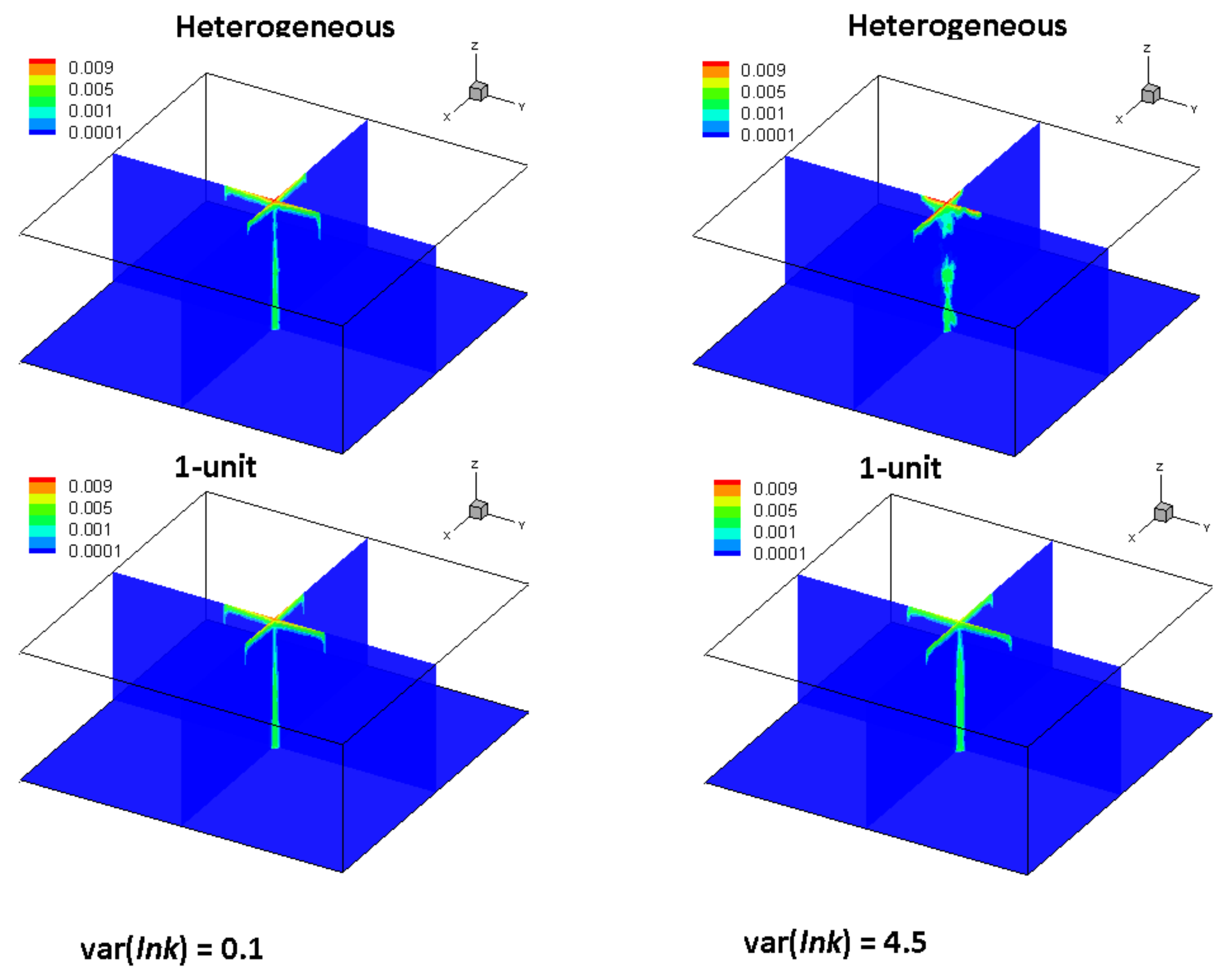
- The reactions between cations and CO_2 forms carbonate minerals (e.g., siderite, magnesite and ankerite) to trap CO_2 as precipitates.

Changes in Volume Fraction:

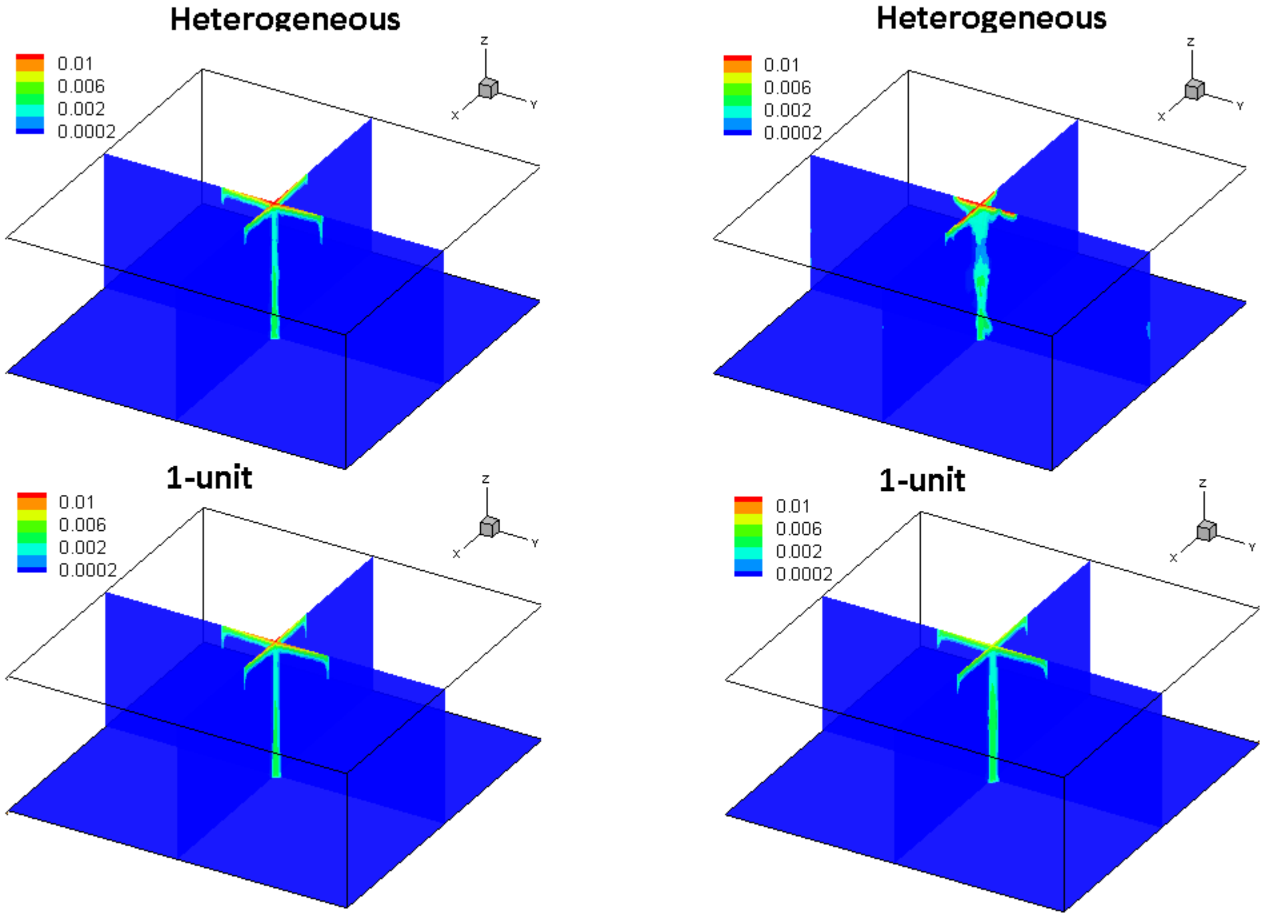
Chlorite after 2000 years



Changes Volume Fraction: Siderite after 2000 years



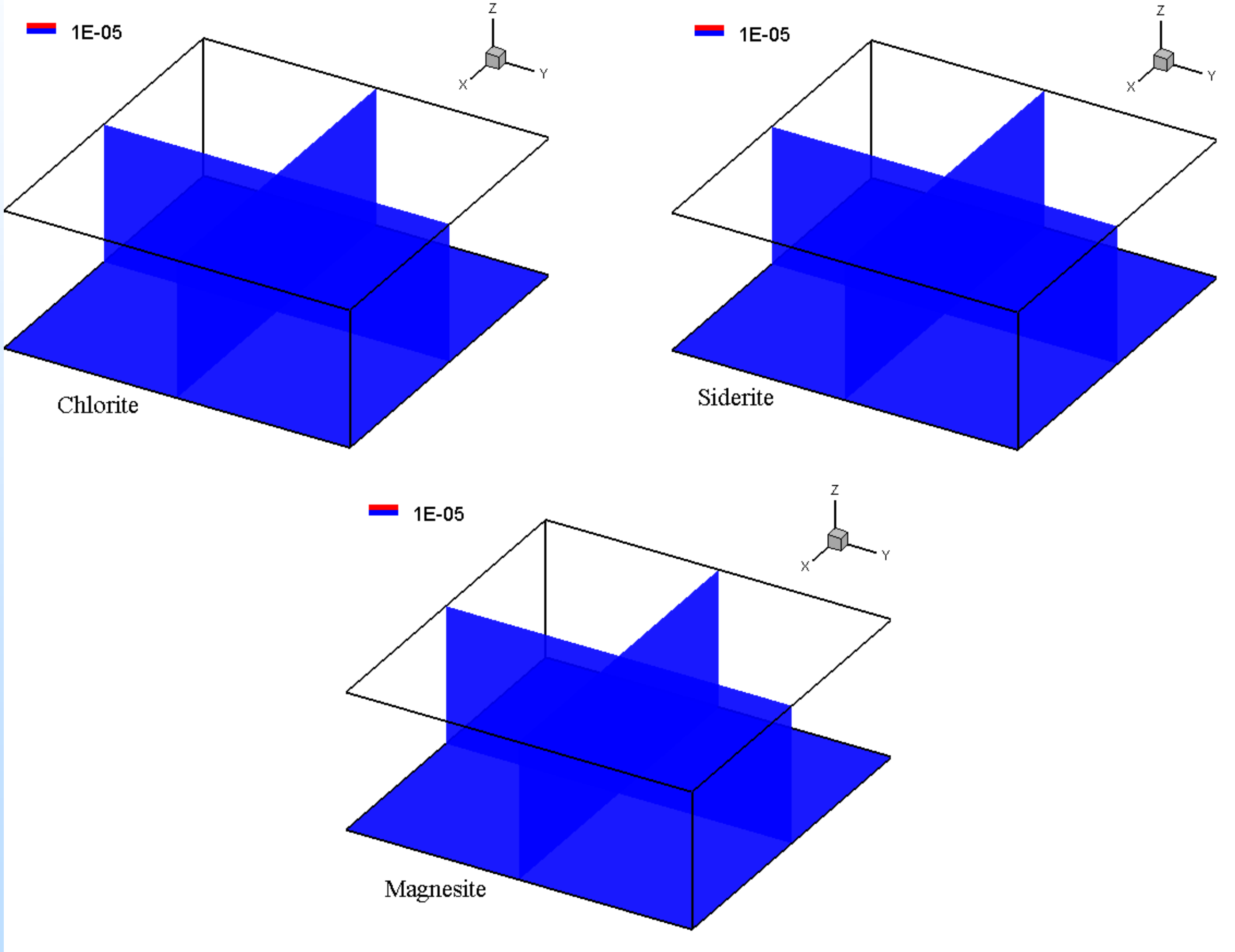
Changes Volume Fraction: Magnesite after 2000 years



var(*lnk*) = 0.1

var(*lnk*) = 4.5

Changes Volume Fraction: without Chlorite after 2000 years



Summary

- Global upscaling computes equivalent *k*s for the geologic models with decreasing k resolution; for increasing reservoir ln(*k*) variances (0.1, 1.0, 4.5), FHM pressure and flow rate are captured well by the geologic models, but errors increase with variance.

- When the variance of ln(*k*) is low, the 1-unit model yields similar dissolution fingering as the FHM. When the variance of ln(*k*) is high, the 1-unit predicts more dissolution fingering per unit time (more optimistic dissolution storage estimate).

- Experimental design analysis suggests that brine salinity is the single most influential factor impacting CO_2 dissolution storage.

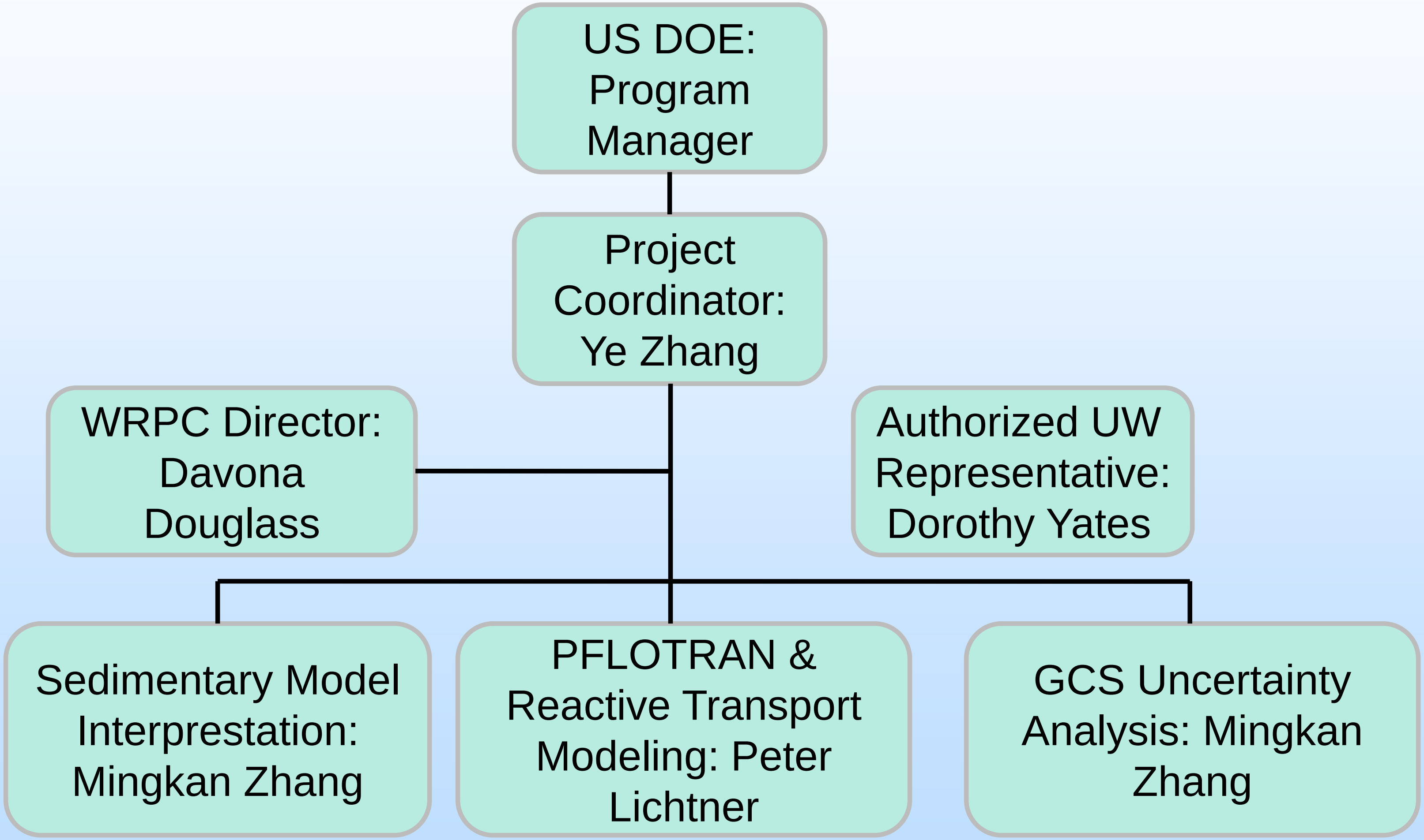
- Reactions between cations and CO_2 forms carbonate mineral precipitates (i.e., Siderite and Magnesite), leading to mineral storage. But, high degree of uncertainty exists in its prediction.

- Next step: For low and high variance systems, complete the DoE and RS analysis for all models with reactions to compare their parameter sensitivity & prediction uncertainty.

Appendix

- These slides will not be discussed during the presentation, but are mandatory

Organization Chart



US DOE: Program Manager

Project Coordinator: Ye Zhang

WRPC Director: Davona Douglass

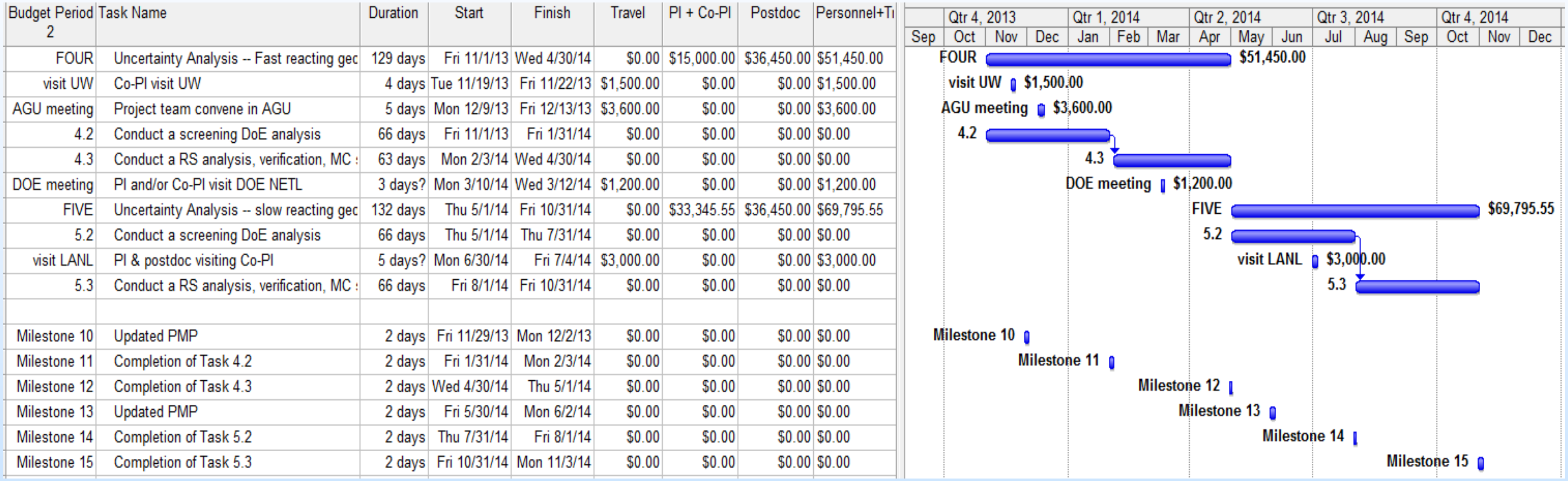
Authorized UW Representative: Dorothy Yates

Sedimentary Model Interprestation: Mingkan Zhang

PFLOTRAN & Reactive Transport Modeling: Peter Lichtner

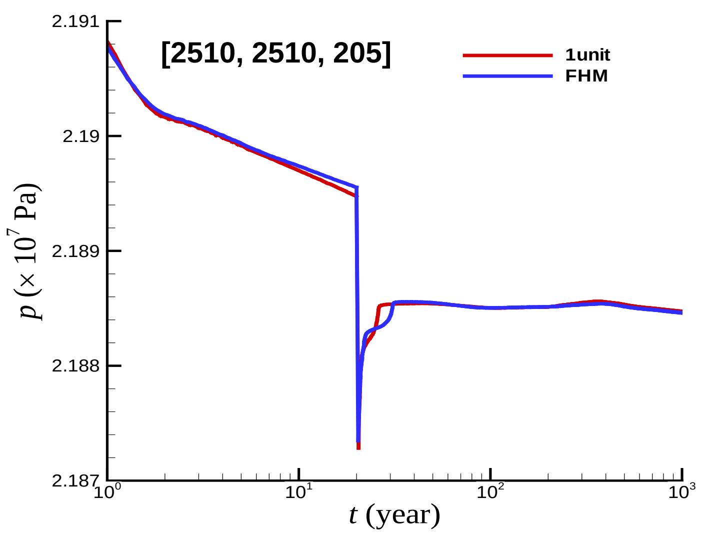
GCS Uncertainty Analysis: Mingkan Zhang

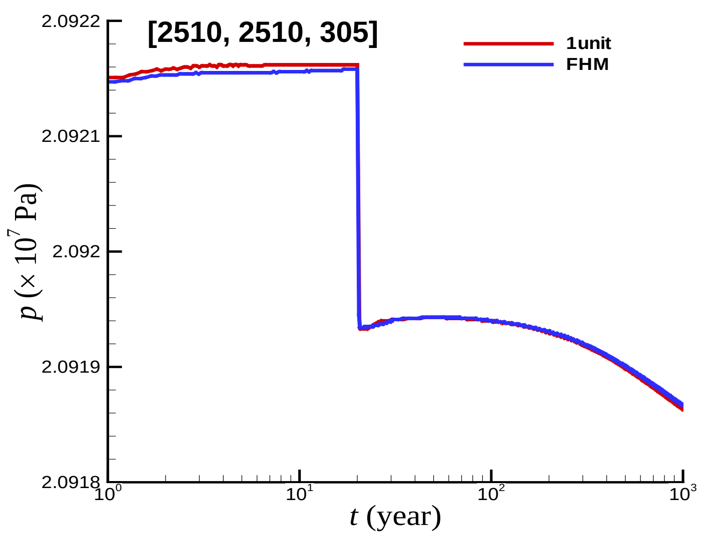
Gantt Chart

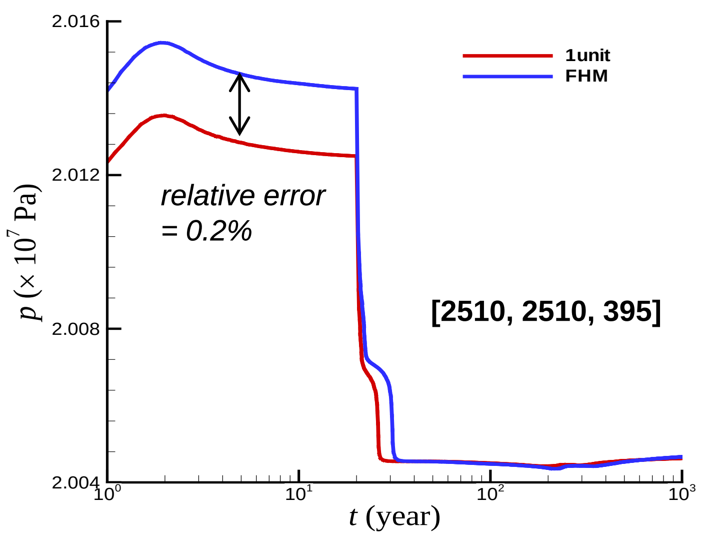


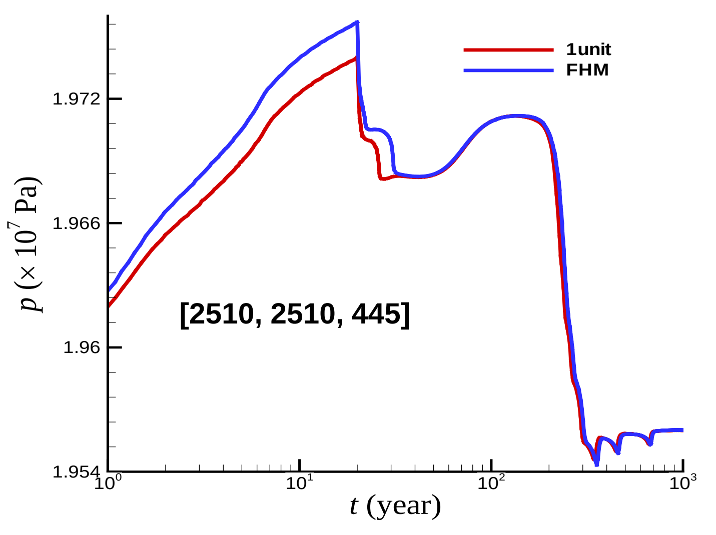
Budget Period 2	Task Name	Duration	Start	Finish	Travel	PI + Co-PI	Postdoc	Personnel+Ti
FOUR	Uncertainty Analysis -- Fast reacting gec	129 days	Fri 11/1/13	Wed 4/30/14	$0.00	$15,000.00	$36,450.00	$51,450.00
visit UW	Co-PI visit UW	4 days	Tue 11/19/13	Fri 11/22/13	$1,500.00	$0.00	$0.00	$1,500.00
AGU meeting	Project team convene in AGU	5 days	Mon 12/9/13	Fri 12/13/13	$3,600.00	$0.00	$0.00	$3,600.00
4.2	Conduct a screening DoE analysis	66 days	Fri 11/1/13	Fri 1/31/14	$0.00	$0.00	$0.00	$0.00
4.3	Conduct a RS analysis, verification, MC	63 days	Mon 2/3/14	Wed 4/30/14	$0.00	$0.00	$0.00	$0.00
DOE meeting	PI and/or Co-PI visit DOE NETL	3 days?	Mon 3/10/14	Wed 3/12/14	$1,200.00	$0.00	$0.00	$1,200.00
FIVE	Uncertainty Analysis -- slow reacting gec	132 days	Thu 5/1/14	Fri 10/31/14	$0.00	$33,345.55	$36,450.00	$69,795.55
5.2	Conduct a screening DoE analysis	66 days	Thu 5/1/14	Thu 7/31/14	$0.00	$0.00	$0.00	$0.00
visit LANL	PI & postdoc visiting Co-PI	5 days?	Mon 6/30/14	Fri 7/4/14	$3,000.00	$0.00	$0.00	$3,000.00
5.3	Conduct a RS analysis, verification, MC	66 days	Fri 8/1/14	Fri 10/31/14	$0.00	$0.00	$0.00	$0.00
Milestone 10	Updated PMP	2 days	Fri 11/29/13	Mon 12/2/13	$0.00	$0.00	$0.00	$0.00
Milestone 11	Completion of Task 4.2	2 days	Fri 1/31/14	Mon 2/3/14	$0.00	$0.00	$0.00	$0.00
Milestone 12	Completion of Task 4.3	2 days	Wed 4/30/14	Thu 5/1/14	$0.00	$0.00	$0.00	$0.00
Milestone 13	Updated PMP	2 days	Fri 5/30/14	Mon 6/2/14	$0.00	$0.00	$0.00	$0.00
Milestone 14	Completion of Task 5.2	2 days	Thu 7/31/14	Fri 8/1/14	$0.00	$0.00	$0.00	$0.00
Milestone 15	Completion of Task 5.3	2 days	Fri 10/31/14	Mon 11/3/14	$0.00	$0.00	$0.00	$0.00

FHM v. 1-Unit Model: $\sigma^2_{\ln k}=0.1$

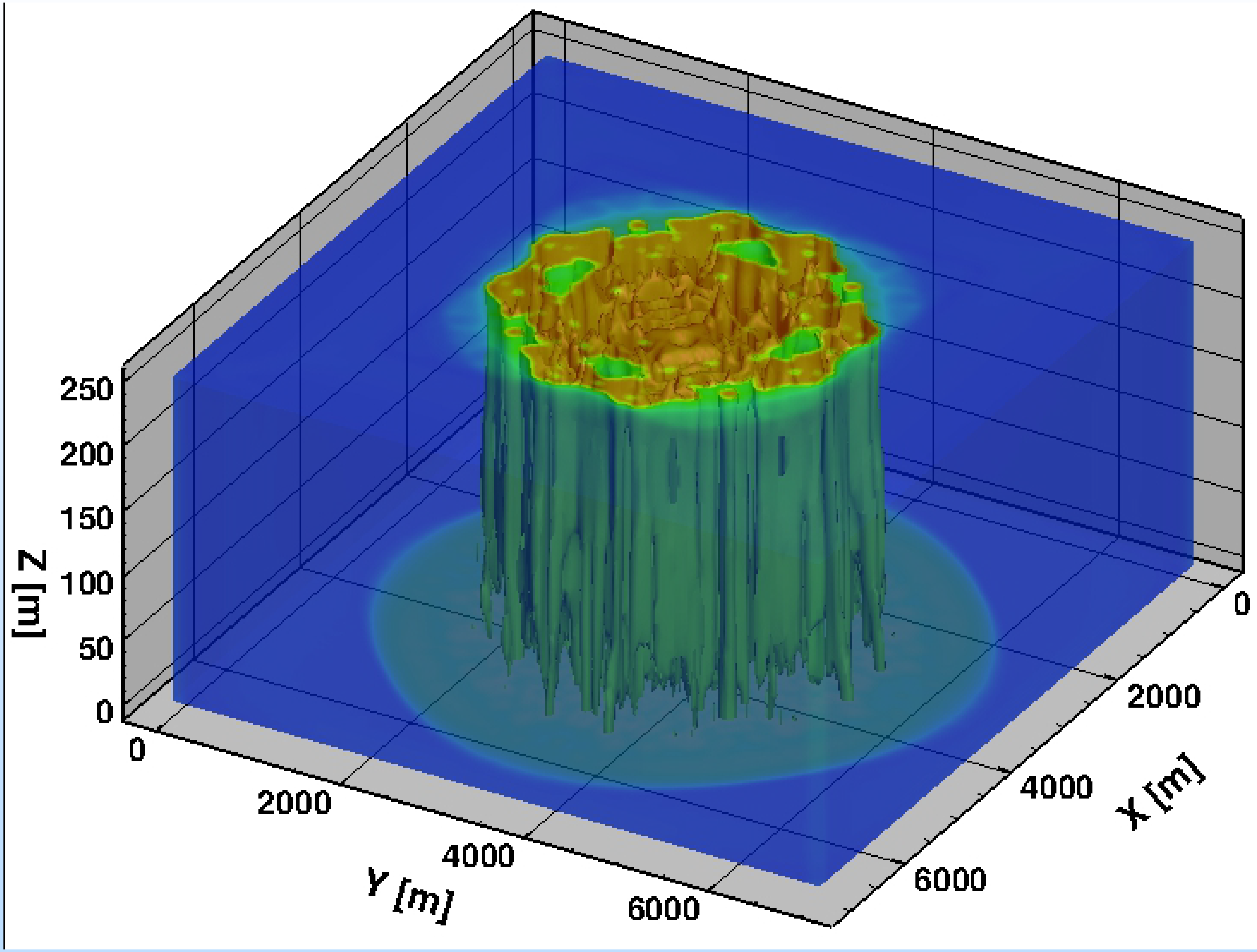




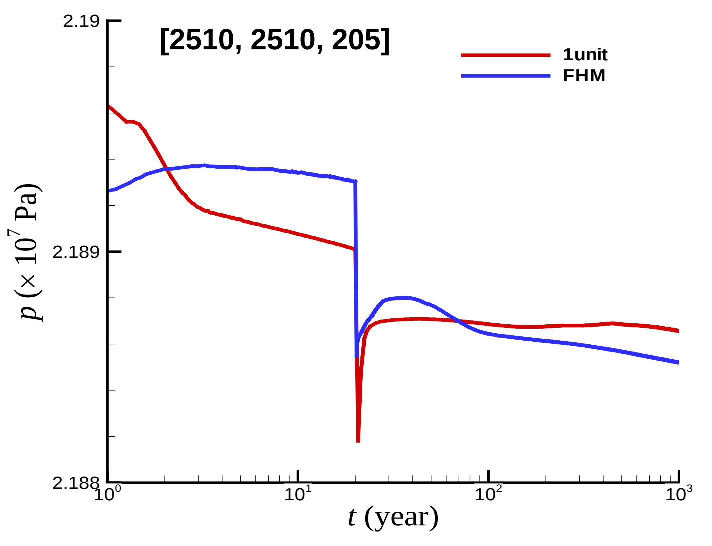


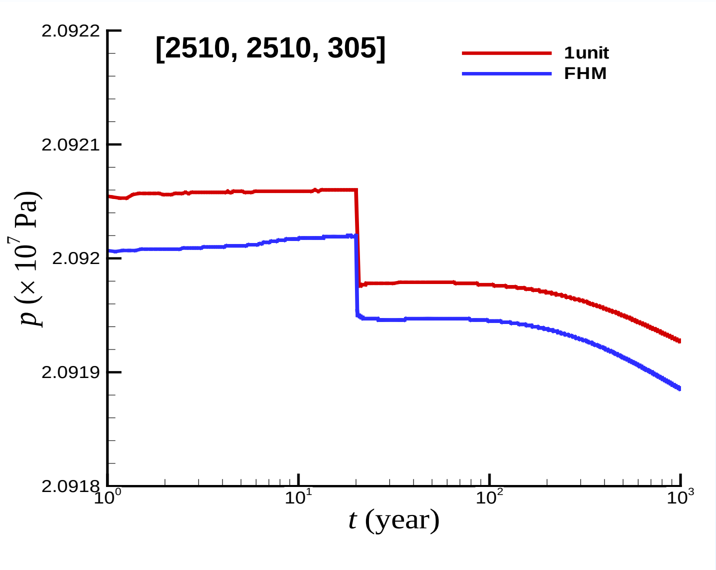


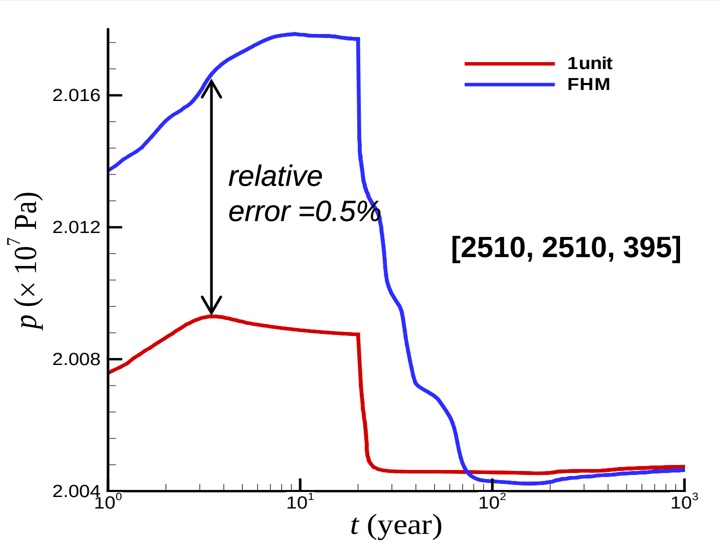
An *example 1-Unit model* run for CO2 storage modeling simulated on the Yellowstone supercomputer. The problem domain is 7000 m x 7000 m x 250 m. Shown at 100 years for an isosurface of 0.0125 (mole fraction) of dissolved CO2. CO2 is injected at a depth of 50 m below the top at the center of the xy-domain for 20 years. The grid is 160 x 160 x 25 =0.64 million cells.



FHM v. 1-Unit Model: $\sigma^2_{\ln k}=4.5$







relative error =0.5%

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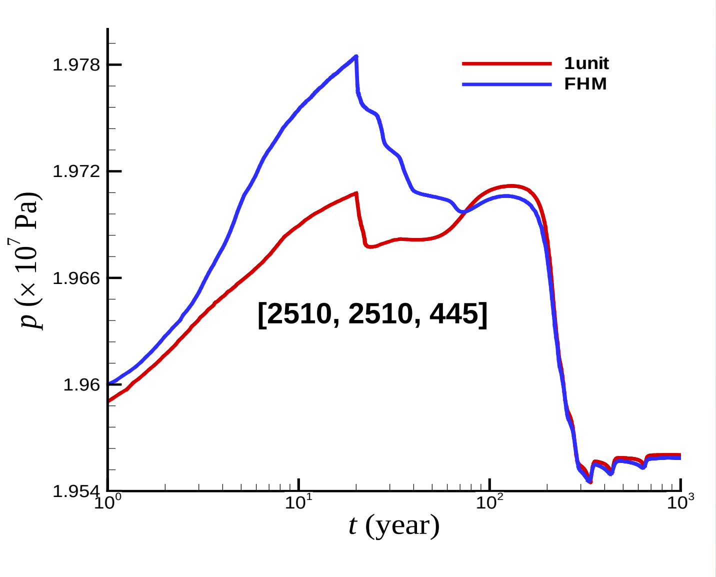
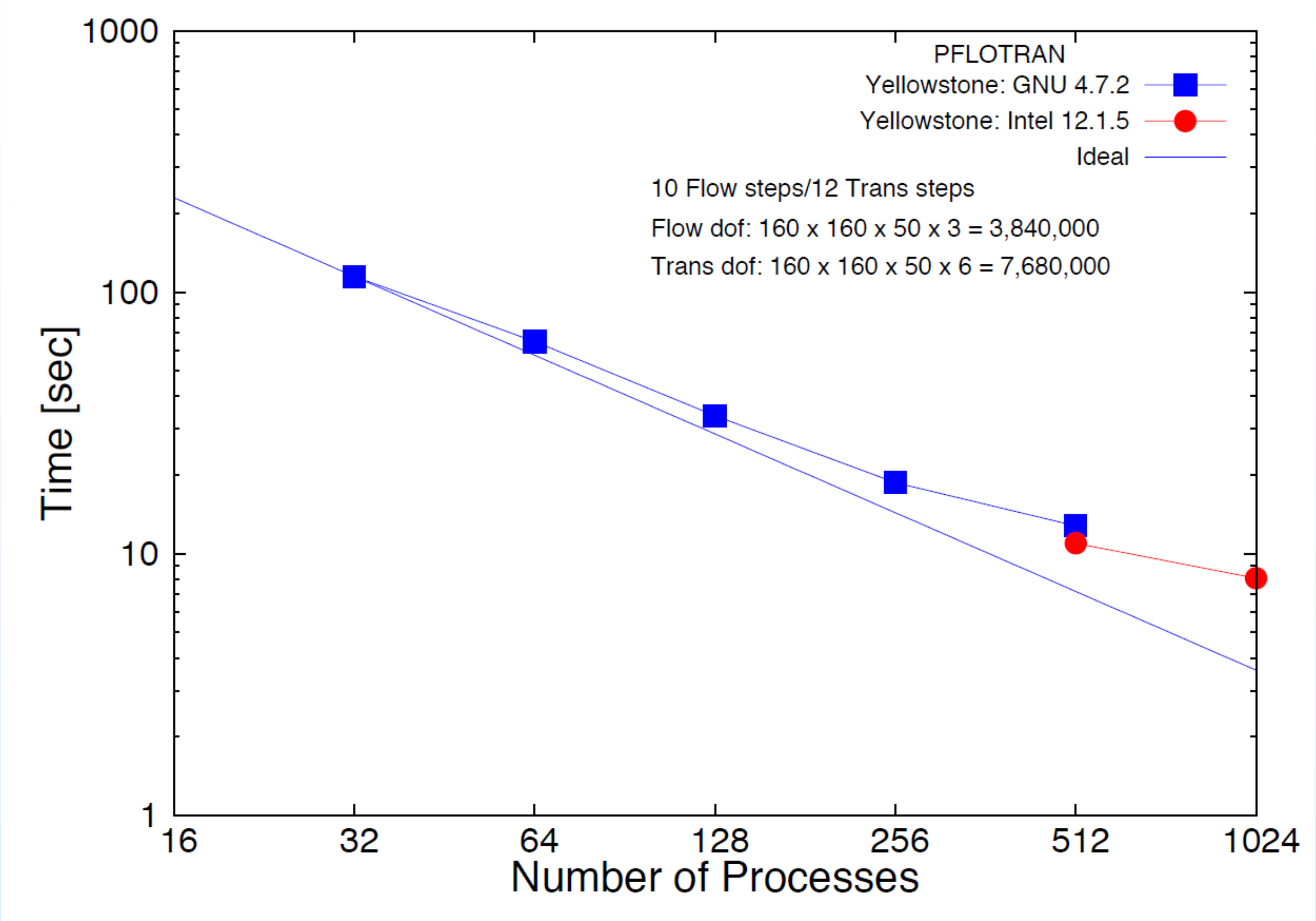


PFLOTRAN Scaling on Yellowstone



PFLOTRAN formulations

To model GCS, the following mass and energy conservation equations are solved:

$$\frac{\partial}{\partial t}\left[\varphi \sum_{\alpha} (\rho_\alpha s_\alpha X_i^\alpha)\right] + \nabla \cdot \sum_{\alpha} (\rho_\alpha X_i^\alpha \vec{q}_\alpha - \varphi \rho_\alpha s_\alpha \tau_\alpha D_\alpha \nabla X_i^\alpha) = S_i \qquad (1)$$

$$\frac{\partial}{\partial t}\left[\varphi \sum_{\alpha} (\rho_\alpha s_\alpha U_\alpha) + (1-\varphi)\rho_r C_{p,r} T\right] + \nabla \cdot \left[\sum_{\alpha} (\vec{q}_\alpha \rho_\alpha H_\alpha) - \lambda \nabla T\right] = Q \qquad (2)$$

φ denotes porosity, and $\rho_\alpha, s_\alpha, \tau_\alpha, D_\alpha, U_\alpha, H_\alpha$ refer to the density, saturation, tortuosity, diffusion coefficient, internal energy, and enthalpy of fluid phase α, respectively. Two fluid phases (CO_2, brine) will be modeled. The quantities X_i^α denote the mole fraction of component *i* in phase α. The quantities $C_{p,r}$ and λ denote the rock heat capacity and conductivity, respectively. The summation is carried out over all fluid phases present in the system. The system is assumed locally to be in thermodynamic equilibrium with temperature $T(\vec{x}; t)$ at position $\vec{x}$ and time *t*. The quantity *Q* denotes an energy source/sink term.

The quantity *Si* denotes a source/sink term for the *i*th primary species describing reaction with minerals given by $S_i = -\sum_m v_{im} I_m$, with stoichiometric reaction coefficients v_{im} and kinetic rate I_m for the *m*th mineral, taken as positive for precipitation and negative for dissolution.

The flow rate $\vec{q}_\alpha$ of fluid phase α is given by the extended Darcy's law: $\vec{q}_\alpha = -\frac{\bar{\bar{k}} k_\alpha}{\mu_\alpha}(\nabla p_\alpha - \rho_\alpha g z)$, with intrinsic permeability $\bar{\bar{k}}$, relative permeability k_α, fluid viscosity μ_α, and pressure p_α of phase α.